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connection with Application No. PP 3804 for a patent by BIOMOLECULAR
RESEARCH INSTITUTE LIMITED filed on 29 May 1998.

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AUSTRALIA

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PROVISIONAL SPECIFICATION

Invention Title:

EGF RECEPTOR AGONISTS AND ANTAGONISTS

The invention is described in the following statement:

EGF RECEPTOR AGONISTS AND ANTAGONISTS

Field of the Invention

This invention relates to the field of epidermal growth factor (EGF) receptor structure and EGF receptor/ligand interactions. In particular, it relates to the field of using the EGF receptor structure to select and screen for agonists and antagonists of the polypeptide ligands.

Background of the Invention

Epidermal growth factor is a small polypeptide cytokine that stimulates marked proliferation of epithelial tissues and is a member of a larger family of structurally related cytokines such as transforming growth factor α (TGF α), amphiregulin, betacellulin, heparin-binding EGF and some viral gene products. Abnormal EGF family signalling is a characteristic of certain cancers (Soler, C. & Carpenter, G., 1994 In Nicola, N. (ed) Guidebook to Cytokines and Their receptors", Oxford Univ. Press, Oxford, pp194-197; Walker, F. & Burgess, A. W., 1994, In Nicola, N. (ed) Guidebook to Cytokines and Their receptors", Oxford Univ. Press, Oxford, pp198-201).

The epidermal growth factor receptor (EGFR) is the cell membrane receptor for EGF (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). The EGFR also binds other ligands that contain amino acid sequences classified as the EGF-like motif. Among these ligands, the three-dimensional structures of EGF and TGF α have been determined by NMR (Montelione, G.T.; Wuthrich, K.; Nice, E.C., Burgess, A.W. and Scheraga, H.A. (1986) *PNAS* 83(22): 8594-8; Campbell, I.D., Cooke, R.M., Baron, M., Harvey, T.S., and Tappin, M.J. (1989) *Prog. Growth Factor Res.* 1, 13-22). Upon binding of the ligand to the extracellular domain, the EGFR undergoes dimerization, which eventually leads to the activation of its cytoplasmic protein tyrosine kinase (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). The EGFR is also known as the ErbB-1 receptor and belongs to the type I family of receptor tyrosine kinases (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-212). This group also includes the ErbB-2, ErbB-3 and ErbB-4 receptors. The ligand of ErbB-2 is still unknown but it is clear that heregulin is binding to ErbB-3 and ErbB-4 (Plowman, G.D., Green, J.M., Calouscou, J.M., Carlton, G.W., Rothwell, V.M., and Buckley, S. (1993) *Nature* 366, 473-475). One of the heregulins is known as neuregulin or NDF and contains an EGF-like sequence that was found to fold into an EGF-like fold by NMR (Nagata, K., Kohda, D., Hatanska, H., Ichikawa, S., Matsuda, S., Yamamoto, T., Suzuki,

A., and Inagaki, F. (1994) *EMBO J.* 13, 3517-3523 and Jacobson, N.E., Abadl, N., Sliwkowski, M.X., Reilly, D., Skelton, N.J., and Fairbrother, W.J. (1996) *Biochemistry* 36, 3402-3417).

The type II family of receptor tyrosine kinases consists of the insulin
 5 receptor (INSR), the insulin-like growth factor I receptor, and the insulin
 receptor-related receptor (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61, 203-
 212). Although the type II receptors consist of four chains ($\alpha_2\beta_2$), both the
 extracellular portions of the receptors from the two families, as well as the
 tyrosine kinase portions, share significant sequence homology, suggesting a
 10 common evolutionary origin (Ullrich, A., and Schlessinger, J. (1990) *Cell* 61,
 203-212, and Bajaj, M., Waterfield, M.D., Schlessinger, J., Taylor, W.R., and
 Blundell, T. (1987) *Biochim. Biophys. Acta* 916, 220-226).

The 621 amino acid residues of the extracellular domain of the human
 EGFR (sEGFR) can be subdivided into four domains as follows: L1, S1, L2
 15 and S2, where L and S stand for "large" and "small" domains, respectively
 (Bajaj, M., Waterfield, M.D., Schlessinger, J., Taylor, W.R., and Blundell, T.
 (1987) *Biochim. Biophys. Acta* 916, 220-226, see Fig. 2). The L1 and L2
 domains are homologous, as are the S1 and S2 domains.

Ligand-induced dimerization was first reported for the EGF receptor
 20 (Schlessinger, J. (1980) *Trends Biochem Sci* 13, 443-447) and now is widely
 accepted as a general mechanism for the transmission of growth stimulatory
 signals across the cell membrane. Although many biochemical experiments
 have been performed to reveal the molecular mechanism of receptor
 dimerization (Lemmon, M.A., Bu, Z., Ladbury, J.E., Zhou, M., Pinchasi, D.,
 25 Lax, L., Engelman, D.M., and Schlessinger, J. (1997) *EMBO J.* 16, 281-294 and
 Tzabar, E., Pinkas-Kramarski, R., Moyer, J.D., Klapper, D.N., Alroy, L.,
 Levkowitz, G., Shelly, M., Henis, S., Eisenstein, M., Ratzkin, B.J., Sela, M.,
 Andrews, G.C., and Yarden, Y. (1997) *EMBO J.* 16, 4938-4950 and Lax, L.,
 Mitra, A.K., Ravern, C., Hurwitz, D.R., Rubinstein, M., Ullrich, A., Stroud,
 30 R.M., and Schlessinger, J. (1991), *J. Biol. Chem.* 266, 13828-13833), the
 molecular mechanism by which monomeric ligands induce dimerization is
 still unknown for members of the EGFR family. Single particle averaging of
 electron microscopic images suggests that the overall shape of the sEGFR is
 four-lobed and doughnut-like (Lax, L., Mitra, A.K., Ravern, C., Hurwitz, D.R.,
 35 Rubinstein, M., Ullrich, A., Stroud, R.M., and Schlessinger, J. (1991), *J. Biol.*
Chem. 266, 13828-13833). Small angle x-ray scattering also indicate that the

sEGFR is a flattened sphere with long diameters of 110 Å and a short diameter of 20 Å (Lemmon, M.A., Bu, Z., Ladbury, J.E., Zhou, M., Pinchasi, D., Lax, L., Engelman, D.M., and Schlessinger, J. (1997) *EMBO J.* 16, 281-294). The crystallization of sEGFR in complex with EGF has been published
 5 (Günther, N., Betzel, C., and Weber, W. (1990) *J. Biol. Chem.* 265, 22082-22085), but the structure has not yet been reported, despite a decade of effort by many groups.

The EGF receptor ligand, TGF- α has been observed to be overproduced in keratinocyte cells which are subject to psoriasis (Turbitt, M.L. et al., 1990,
 10 *J. Invest. Dermatol.* 95(2), 229-232; Higashimiyama, M. et al., 1991, *J. Dermatol.*, 18(2), 117-119; Elder, J.T. et al, 1990, 94(1), 19-25). The overproduction of at least one other EGF receptor ligand, amphiregulin, has also been implicated in psoriasis. (Piepkorn, M. 1996, *Am. J. Dermatopath.*, 18(2), 165-171). Molecules that inhibit the EGF receptor have been shown to
 15 inhibit the proliferation of both normal keratinocytes (Dvir, A. et al, 1991, *J. Cell Biol.*, 113(4), 857-865) and psoriatic keratinocytes. (Ben-Bassat, H. et al., 1995, *Exp. Dermatol.*, 4(2), 82-88). These findings indicate that EGF receptor antagonists may be useful in the treatment of psoriasis.

Many cancer cells express constitutively active EGFR (Sandgreen, E. P., et al., 1990, *Cell*, 61:1121-135; Karnes, W. E. J., et al., 1992, *Gastroenterology*, 102:474-485) or other EGFR family members (Hynes, N. E., 1993, *Semin. Cancer Biol.* 4:19-26). Elevated levels of activated EGFR occur in bladder, breast, lung and brain tumours (Harris, A. L., et al., 1989, In
 20 Furth & Greaves (eds) *The Molecular Diagnostics of human cancer*. Cold Spring Harbor Lab. Press, CSH, NY, pp353-357). Antibodies to EGFR can inhibit ligand activation of EGFR (Sato, J. D., et al., 1983 *Mol. Biol. Med.* 1:511-529) and the growth of many epithelial cell lines (Aboud-Pirak E., et al., 1988, *J. Natl Cancer Inst.* 85:1327-1331). Patients receiving repeated doses of a humanised chimeric anti-EGFR monoclonal antibody (Mab) showed
 25 signs of disease stabilization. The large doses required and the cost of production of humanised Mab is likely to limit the application of this type of therapy. These findings indicate that the development of EGF receptor antagonists will be attractive anticancer agents.

Summary of the Invention

The present inventors have now obtained 3-dimensional structural information concerning the epidermal growth factor receptor (EGFR). This structural information was obtained by comparative modelling based on the 3D structure of the IGF-1 receptor as described in PP0585 and PP2598 (a copy of which is annexed hereto as Annexure A). The information presented in the present application provides the opportunity for the development of specific antagonists and agonists of EGFR for therapeutic applications.

Accordingly, in a first aspect the present invention provides a method of screening for, or designing, an agonist of the EGF receptor which method includes

(i) selecting or designing a substance which possesses stereochemical complementarity to the EGF receptor site, wherein the receptor site is characterised by

(a) amino acids 1-474 of the EGF receptor positioned at atomic coordinates substantially as shown in Figure 6 and 7 or a subset thereof; and

(ii) testing the substance for the ability to act as an agonist of the EGF receptor.

In a second aspect the present invention provides a method of screening for, or designing, an antagonist of the EGF receptor which method includes

(i) selecting or designing a substance which possesses stereochemical complementarity to the EGF receptor site, wherein the receptor site is characterised by

(a) amino acids 1-474 of the EGF receptor positioned at atomic coordinates substantially as shown in Figures 6 and 7 or a subset thereof; and

(ii) testing the substance for the ability to act as an antagonist of the EGF receptor.

The EGF receptor site defined in the first and second aspects of the present invention comprises the L1, S1 and L2 domains (residues 1-474) of the ectodomain of EGFR. At the centre of this structure is a cavity, bounded by all three domains, of sufficient size to accommodate a ligand molecule. By "stereochemical complementarity" we mean that the substance or a portion thereof correlates, in the manner of the classic "lock-and-key" visualisation of ligand-receptor interaction, with the cavity in the receptor site. Preferably, the stereochemical complementarity is such that the

substance has a K_i for the receptor site of less than $10^{-6}M$. More preferably, the K_i value is less than $10^{-8}M$ and more preferably less than $10^{-9}M$.

In preferred embodiments of the first and second aspects of the present invention, the method further involves selecting or designing a substance
5 which has portions that match residues positioned on the surface of the receptor site which faces the cavity. By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by enthalpy-reducing Van der Waals interactions which promote desolvation of the biologically active substance within the site, in such a way
10 that retention of the substance within the cavity is favoured energetically.

In a preferred embodiment of the first aspect of the present invention, the method includes screening for, or designing, a substance which possesses a stereochemistry and/or geometry which allows it to interact with both the L1 and L2 domains of the EGF receptor site. It is believed that EGFR
15 monomers dimerise in nature in such a manner that the cavities of each monomer may face each other. Accordingly, the method of the first aspect of the present invention may involve screening for, or designing, a biologically active substance which interacts with the L1 domain of one monomer and the L2 domain of the other monomer.

20 In a third aspect the present invention provides a method of selecting or designing an agonist of the EGF receptor which method includes

- (i) selecting or designing a substance which interacts with
 - (a) a fragment of the EGF receptor characterised by amino acids 1-474 positioned at atomic coordinates substantially as shown in Figures 6
25 and 7 or a subset thereof;

wherein the interaction of the substance with the fragment alters the position of at least one of the L1, L2 or S1 domains of the fragment relative to the position of at least one of the other domains; and

- (ii) testing the substance for the ability to act as an agonist of the EGF
30 receptor.

In a preferred embodiment of the third aspect of the present invention the substance interacts with the fragment in the region of the L1 domain-S1 domain interface, causing the L1 and S1 domains to move away from each other. In a further preferred embodiment the substance interacts with the
35 hinge region between the L2 domain and the S1 domain causing an alteration in the positions of the domains relative to each other. In a further preferred

embodiment the substance interacts with the β sheet of the L1 domain causing an alteration in the position of the L1 domain relative to the position of the S1 domain or L2 domain.

In a fourth aspect the present invention provides an agonist of the EGF receptor obtained by a method according to the first or third aspects of the present invention.

In a fifth aspect the present invention provides an antagonist of the EGF receptor obtained by a method according to the second aspect of the present invention.

The agonists or antagonists of the fourth and fifth aspects of the present invention may be mutant EGFR ligands where at least one mutation occurs in the region of the ligand which interacts with residues on the surface of the receptor site facing toward the cavity. For example, the residues Arg 41 and Tyr 13 in EGF are conserved in other members of the EGF receptor family of ligands (a Phe residue may be substituted for Tyr 13). Structures of several EGF family members show the two residues to be in close proximity. This portion of EGF may interact with a hydrophobic portion of the EGF receptor which contains one or more negatively charged residues such as the lower β sheet of the L1 domain. Mutants of EGF which show altered activity may be generated by introducing modifications to Arg 41 or Tyr 13 or other nearby residues. Alternatively, mutants of EGF may be generated by introducing modifications to residues on the opposite side of the ligand which may interact with a second receptor molecule in the unmodified ligand.

In a sixth aspect the present invention provides a substance which possesses stereochemical complementarity to the EGF receptor site, wherein the receptor site is characterised by

(a) amino acids 1-474 of the EGF receptor positioned at atomic coordinates substantially as shown in Figures 6 and 7 or a subset thereof;

with the proviso that the substance is not a naturally occurring ligand of the EGF receptor or a mutant thereof.

By "mutant" we mean a ligand which has been modified by one or more point mutations, insertions of amino acids or deletions of amino acids.

In a preferred embodiment of the sixth aspect of the present invention, the stereochemical complementarity is such that the compound has a K_i for

the receptor site of less than 10^{-6} M. More preferably, the K_i value is less than 10^{-8} M and more preferably less than 10^{-9} M.

The 3 dimensional structure of the EGF receptor elucidated by the present inventors also shows that the L2 and S2 domains are positioned such that they form a "corner" structure. It is envisaged that this corner structure provides a further binding site for ligands of the EGF receptor.

Accordingly, in a seventh aspect the present invention provides a method of screening for, or designing, an agonist of the EGF receptor which method includes

- (i) selecting or designing a substance which binds simultaneously to the L2 and S2 domains of the EGF receptor, wherein the L2 and S2 domains are positioned substantially according to the atomic coordinates of amino acids 313-621 as shown in Figure 7, and
- (ii) testing the substance for the ability to act as an agonist of the EGF receptor.

In an eighth aspect the present invention provides a method of screening for, or designing, an antagonist of the EGF receptor which method includes

- (i) selecting or designing a substance which binds simultaneously to the L2 and S2 domains of the EGF receptor, wherein the L2 and S2 domains are positioned substantially according to the atomic coordinates of amino acids 313-621 as shown in Figure 7, and
- (ii) testing the substance for the ability to act as an antagonist of the EGF receptor.

In preferred embodiments of the seventh and eighth aspects of the present invention, the method involves selecting or designing a substance which has portions that match residues positioned on the inner surface of the corner structure. By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by enthalpy-reducing Van der Waals interactions in such a way that retention of the substance within the corner structure is favoured energetically.

Preferably, the substance matches the residues positioned on the inner surface such that the substance has a K_i for the corner structure of less than 10^{-6} M. More preferably, the K_i value is less than 10^{-8} M and more preferably less than 10^{-9} M.

In a ninth aspect the present invention provides a method of selecting or designing an agonist of the EGF receptor which method includes

- (i) selecting or designing a substance which interacts with
 - (a) a fragment of the EGF receptor characterised by amino acids 313-621 positioned at atomic coordinates substantially as shown in Figure 7 or a subset thereof;

wherein the interaction of the substance with the fragment alters the relative positions of the L2 and S2 domains of the fragment with respect to each other; and

- (ii) testing the substance for the ability to act as an agonist of the EGF receptor.

In a tenth aspect the present invention provides an agonist of the EGF receptor obtained by a method according to the seventh or ninth aspects of the present invention.

- In an eleventh aspect the present invention provides an antagonist of the EGF receptor obtained by a method according to the eighth aspect of the present invention.

- In a twelfth aspect the present invention provides a pharmaceutical composition for preventing or treating a disease which would benefit from increased signalling by the EGF receptor, which includes an agonist obtained by a method according to the first, third, seventh or ninth aspects of the present invention and a pharmaceutically acceptable carrier or diluent.

- In an thirteenth aspect the present invention provides a pharmaceutical composition for preventing or treating a disease associated with signalling by the EGF receptor which includes an antagonist obtained by a method according to the second or eighth aspects of the present invention and a pharmaceutically acceptable carrier or diluent.

- In a fourteenth aspect the present invention provides a method of preventing or treating a disease which would benefit from increased signalling by the EGF receptor which method includes administering to a subject in need thereof an agonist obtained by a method according to the first, third, seventh or ninth aspects of the present invention.

Diseases which may be treated by administration of EGFR agonists include wound healing and gastric ulcers.

- In a fifteenth aspect the present invention provides a method of preventing or treating a disease associated with signalling by the EGF

receptor which method includes administering to a subject in need thereof an antagonist obtained by a method according to the second or eighth aspects of the present invention.

Diseases associated with signalling by the EGF receptor include psoriasis and many types of tumour states including but not restricted to cancer of the breast, brain, ovary, cervix, pancreas, lung, head and neck, and melanoma, rhabdomyosarcoma, mesothelioma and glioblastoma.

Brief Description of the Drawings

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Figure 1: Sequence alignment of human EGF receptor family proteins with IGF-1 receptor sequences and insulin receptor sequence for the first two domains of the EGF receptor. The alignment of EGF receptor and the various IGF-1 receptor sequences were used by the MODELLER program to create a model of the EGF receptor domains L1 and S1. Residues which are underlined were used to create additional α - α restraints for the construction of the EGF receptor model. IGF-1 receptor residues colored in magenta form part of helical secondary structures. Residues colored in light blue, light green and dark yellow reside in one of the three β -sheets (colored light blue, light green and dark yellow respectively) which make up part of the L1 β -helix. Residues colored in dark blue and dark green form part of a β -strand in the β -fingers. The residues in red are also in β -strands. Each cysteine residue in the S1 domain are numbered according to the module that it is a part of.

25

Figure 2: Sequence alignment of human EGF receptor family proteins with IGF-1 receptor sequences and insulin receptor sequence for the third and fourth domains of the EGF receptor. The labelling scheme of the residues is the same as for Figure 1.

30

Figure 3: Model polypeptide fold of the L1 and S1 domains of the EGF receptor. The L1 domain is at the left hand side of the structure with the N-terminus facing the front. The secondary structure elements are coloured in the same manner as in Figure 1.

35

Figure 4: Model polypeptide fold of the L2 and S2 domains of the EGF receptor. The L2 domain is at the bottom with its N-terminus facing the front. The secondary structure elements are coloured in the same manner as in Figure 1.

5

Figure 5: Superposition of the two models (of L1 and S1 domains and of L2 and S2 domains) onto structure of first three domains of IGF-1 receptor. The residues have been colored according to an estimate of the accuracy of the model coordinates. Residues colored in yellow are judged to be well-modelled. Residues colored in orange are judged to have a moderate possibility of error. The coordinates or residues colored in red are believed to be inaccurate.

10

Figure 6: Coordinates of the model of the EGF receptor domains L1 and S1. The coordinates are in relation to a Cartesian set of orthogonal axes. The final column contains the number 20, 40 or 60 depending on whether the residue containing the atom is judged to be well modelled, have a moderate possibility of error or is believed to be inaccurate respectively.

15

Figure 7: Coordinates of the model of the EGF receptor domains L2 and S2. The coordinates are in relation to a Cartesian set of orthogonal axes which are independent of the coordinate frame used for the EGF receptor model for L1 and S1 domains. The number in the final column is assigned in the same manner as for Figure 6.

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Detailed description of the Invention

Comparative modelling

The comparative modelling method exploits the observation that proteins with more than 25% amino acid identity will almost always have a similar protein backbone (Sander, C. And Schneider, R., 1991, Proteins: Structure Function and Genetics, 9, 56-68). In some cases, proteins will have similar backbone structures with a lower proportion of identical amino acids. By aligning the sequence of a (target) protein which is to be modelled with the sequences with known structures (the templates), a model of the protein can be obtained. Where a region of the target sequence follows the sequences

30

35

of a template, the backbone of the target is built to follow that of the template. Where the target sequence can not be aligned to a target sequence, the so-called insertion must be constructed by other means (Greer, J., 1991, Meth. Enzym. pp 239-252).

5 The MODELLER program (Šali, A and Blundell, T.L., 1993, J. Mol. Biol. 234, 779-815) is a semi-automated approach to building models of proteins given the structures of one or more template structures and an alignment between the sequences of the target protein and the templates. Based on the sequence alignment and a set of rules derived from the analysis
10 of sets of aligned structure, the program generates a series of restraints for variables such as C α -C α distances, main chain and side chain dihedral angles for the target structure. The restraints are expressed in terms of probability density functions (PDFs). The PDFs are combined to yield an expression for the most probable structure as a function of the variables (C α -C α distances
15 etc). The program then attempts to find structures to maximise the value of this function. In effect, the program attempts to minimise a transformed version of this function.

While some comparative modelling approaches involve the explicit building of regions of the model for which there is no sequence alignment
20 with a template, the MODELLER program constructs PDFs for these regions, thus including them in the consideration of constructing a comparative model. It is conceivable that once a comparative model has been constructed using MODELLER that an algorithm to build the structures of these regions is applied.

25 The MODELLER program was used to build the structures of the extracellular portion of the EGF receptor using the 3D structure of the IGF-1 receptor (as described in PP0585 and PP2598) as a template. The description of the generation of these models is outlined below.

Construction of the alignment

30 The sequence of the EGF receptor extracellular domain can be divided into four domains, L1, S1, L2 and S2 on the basis of internal homology and homology with the insulin receptor family (Ward, C.W. et al., 1995, Proteins: Structure Function and Genetics 22: 141-153; Bajaj, M. et al., 1987, Biochim. Biophys. Acta 916: 220-226). At least two important sequence motifs are
35 found in the EGF receptor sequence which are conserved in other EGF receptor homologues. The first motif is the sequence CXXXXXXW which is

found towards the end of both L1 and L2 of EGFR (C is cysteine, W is tryptophan and X is any residue). The second motif is the sequence CW where C is the third cysteine of both S1 and S2 (using the assignment of domain boundaries from Ward, C.W. et al., 1995, *Proteins: Structure* 5 *Function and Genetics* 22: 141-153). The first motif is found in L1 but not L2 of the insulin receptor family. The second motif is found in the cysteine-rich domain of the insulin receptor family. These motifs are found in L1 and the cysteine-rich domain of the insulin receptor family. Structurally, the first motif corresponds to part of the L1 domain which allows penetration of the 10 tryptophan residue of the second motif into the β -helix. As the first sequence motif is absent from L2 of the IGF-1 receptor, only the L1 and cysteine rich domains of the IGF-1 receptor were used as templates for the building of the EGF receptor extracellular domain models.

Construction of the alignment of L1 and S1

15 There are two loops in the structure of the L1 domain which emerge from the breadloaf structure. The second loop (residues 86-93 in EGFR L1, 79-85 in IGF-1R L1) is structurally conserved in the L2 domain and differs by one amino acid residue in length. A region of the L2 domain corresponding to the loop was used as an additional template for this region. The sequence 20 of the EGF receptor which corresponds to the first loop is of a different length and does not seem to be consistent with the loop of the IGF-1 receptor. The latter half of the region of EGF receptor sequence can be aligned to a region of sequence in the IGF-1 receptor's L2 domain. A portion of the IGF-1 receptor structure corresponding to this region of sequence plus the structure 25 of flanking sequences was used as an additional template.

The alignment of the S1 domain of the EGF receptor to the IGF-1 receptor used the same combination of modules but involved the use of other modules from the cysteine-rich domain as additional templates. The first and second modules of the EGF module used the third module of the IGF-1 30 receptor cysteine-rich domain as additional templates. (This module contains two cysteines in disulfide bonds in a 1-3, 2-4 arrangement.) The sixth module of the EGF receptor can be modelled by the fifth module of the IGF-1 receptor, a β -finger.

Construction of the alignment of L2 and S2

35 The alignment of the EGF receptor sequence for the L2 domain to the L1 domain of the IGF-1 receptor sequence was similar to that of the L1

alignment. There is a 16 amino acid region which occurs roughly in the same region as the first loop in the IGF-1 receptor L1 domain. This region of sequence, which exhibits sequence homology amongst the EGF receptor family of proteins, can not be aligned with any region of the IGF-1 receptor sequence.

The sequence of the S2 domain was found to differ significantly from the S1 domain and suggested that the pattern of disulfide bonds may be different.

An analysis of the β -finger structures in the IGF-1 receptor, TNF receptor and laminin- γ structures revealed that the β -fingers could be classed into three types exhibiting some structural and sequence conservation. Two of the structural types are relevant to the IGF-1 and EGF receptors. The first type of β -finger is characterised by structural conservation of the C-terminal portion of the module and also of the linker region after the module. The sequence signature is C...CXXC where the third cysteine residue is the start of another β -finger module. The second type of β -finger is characterised by structural conservation of the N-terminal portion of the module and also of the linker region after the module. The sequence signature is C...CXXXC where the third cysteine is the start of a module whose disulfide bonding pattern is 1-3,2-4. The fifth module of the IGF-1 receptor cysteine-rich domain has some structural conservation with both types of β -finger.

The regions of the IGF receptor structure which were used as templates were identified as follows. The structure of IGF-1 receptor from the start of the L1 domain to the end of the first module of the cysteine-rich domain (which contains the conserved tryptophan residue which intercalates into the L1 β -helix) was used to model the corresponding regions of L2 and the start of S2 of the EGF receptor. Additional templates were used and "joined" to other templates by virtue of overlap in the sequence alignment.

The fourth and fifth modules of the IGF-1 receptor cysteine-rich domain were found to align with the sequences of the first and second and also the fourth and fifth putative modules of the S2 domain. The seventh module is the second last module of the S2 domain. The eighth module is neither a β -finger nor a module with the 1-3, 2-4 pattern of disulfide bonds. By elimination and use of the information described in the preceding paragraph, the third and sixth modules were assigned to be β -fingers of the second type. Two parts of the IGF-1 receptor structure were used to model

these two β -fingers. The fifth and seventh modules were used to model the β -finger modules. The linker region after the seventh module was also used. Additional residues after the linker were included to guide the placement of the next module. The positioning of the next module (modules 4 and 7 in S2) is essentially arbitrary and the use the extra residues offers a way of obtaining a plausible placement of the module.

Construction of the model

Version 3 of the MODELLER program (Modeler User Guide, October 1996, San Diego Molecular Simulations Inc) was used to build models of the EGF receptor. Models of the L1 and S1 domains were constructed from the alignment shown in Figure 1 using the IGF-1 receptor templates shown and the EGF receptor sequence. Additional distance restraints were generated between C α atoms of selected residues. The restraints were generated as follows. The small IGF-1 receptor templates were superimposed into the structure of the first two domains of the IGF-1 receptor using the C α atoms of the residues which are aligned in Figure 1. Using the Homology module of the Insight II program (Homology User Guide, October 1995, San Diego BIOSYM/MSI) coordinates were built for the EGF receptor residues which are aligned to the IGF-1 receptor coordinates which are in bold typeface. From these coordinates, distance restraints in the form of Gaussian curves were constructed for pairs of C α atoms with a distance less than 50Å. The sigma value of the Gaussian curves was set to be 2Å. A MODELLER run was submitted using the alignment in Figure 1. The built models of proteins attempt to satisfy these restraints in addition to the restraints the program derives from the alignment.

To build models of the L2 and S2 domains, a similar process to that described in the preceding paragraph was used. The alignment used to build the models is shown in Figure 2. Two separate sets of additional restraints were used. The first set of restraints were derived from the IGF-1 receptor templates which are aligned with the first, second and third modules of the EGF receptor S2 domain. The second set of restraints were derived from the IGF-1 receptor templates which were aligned with the fourth, fifth and sixth modules of the EGF receptor S2 domain. Only those residues which are underlined in Figure 2 were used to generate the restraints. The sigma value of the Gaussian curves used to construct the additional restraints was 1Å.

For both sets of models, the MODELLER program constructed 20 models whose coordinates were perturbed from an initial structure by a random value of maximum distance 4Å. The refinement level used was the 'refine1' option in the MODELLER program.

5 Structure of the EGF receptor model

The structure of the L1 and S1 domains of the EGF receptor as determined by the modelling described above is shown in Figure 3, while the structure of the L2 and S2 domains is shown in Figure 4. The superposition of these two models onto the structure of the extracellular domains of the IGF-1 receptor is shown in Figure 5.

The coordinates of the EGF receptor domains L1 and S1 are shown in Figure 6. The coordinates of the EGF receptor domains L2 and S2 are shown in Figure 7.

The structures of the L1 and S1 domains are similar to those of the IGF-1 receptor structure, as expected. There are two major differences in the S1 domain from the structure of the cysteine-rich region of the IGF-1 receptor structure. The sixth module of S2 is smaller than that of the IGF-1 receptor and occupies less of the region between the two L domains. The fifth module, another β -finger, contains a large insertion which points away from the L1 domain. The structure of the end of the EGF receptor S1 domain is similar to that of the IGF-1 receptor cysteine-rich domain and is postulated to contain a hinge region between the last module of the S1 domain and the L2 domain.

A region of EGF receptor in L2 which could not be aligned with the IGF-1 receptor sequence includes the amino acids Trp-Pro which are conserved in the EGF receptor family of structure. This sequence motif is not found in the insulin receptor family and may represent a region of novel structure. This region of sequence could not be modelled on the corresponding region of the IGF-1 structure since none of the amino acids of the sequence Glu-Asn-Arg could be placed such that their side chains are in the interior of the β -helix. The asparagine has been observed to be glycosylated (Smith, K.D. et al, 1996, Growth.Factors, 13(1-2), 121-132) and therefore must point out of the structure. The charged residues glutamate and arginine are also expected to point out from the β -helix.

The amino acids 352-367 correspond to a large insertion in the third domain of the EGF receptor. The amino acids 351-364 have been identified as the epitope for several antibodies against the EGF receptor (Wu, D.G et al,

J. Biol. Chem. 1989 264(29):17469-17475). That this region forms a loop which sticks out of the structure is consistent with this region being accessible to the antibodies. The structure itself is difficult to model accurately since its sequence does not correspond to any part of the IGF-1 receptor sequence. The position of this insertion is in approximately the same region where the structures of IGF-1 receptor L1 and L2 domain differ.

The S2 domain adopts a different shape to the S1 domain. The S2 domain adopts a rod-like shape similar to that of the laminin γ -chain (Stetefeld, J. et al., 1996, J. Mol. Biol., 257(3): 644-657). Like the first half of the receptor model, the S2 domain contacts the L2 domain with the first module (this module contains the conserved tryptophan which intercalates into the breadloaf). Unlike S1, the rest of the S2 domain does not make any more contact with the L2 domain. The S2 domain points out from the L2 domain with a different geometry to the manner in which the S1 domain points out from L1.

Putative binding sites of the EGF receptor

From the IGF-1 receptor structure and a number of insulin receptor mutants, one of the regions of insulin binding was proposed to be the lower β sheet of the L1 domain. This surface is characterised by a number of hydrophobic residues which point out of the structure and also the presence of a structurally conserved loop. By analogy, we propose that the analogous β sheets of the L1 and L2 are potential binding sites. These sheets contain a number of hydrophobic residues, conserved amongst EGF receptor family members, which point away from the core of the β -helix structure. Residue 45 of a mutant EGF has been cross-linked to the residue Lysine 465 which is in the last strand of the lower β sheet of the L2 domain. (Summerfield, AE et al, J Biol Chem, 1996, 271(33), 19656-19659). Tyrosine 101 has been cross-linked to the N-terminus of EGF (Woltjer, RL et al, PNAS, 1992, 89(16), 7801-7805). This residue is in the portion of sequence which immediately follows a strand in the lower β sheet of L1.

The side chain of asparagine 1 of EGF has been cross-linked to lysine 336 of the EGF receptor (Wu, DG et al, PNAS, 1990, 87(8), 3151-3155). The latter residue is in the N-terminal helix of the L2 domain and points towards the cavity which is formed when the two halves of the EGF receptor are positioned in a similar arrangement to the first three domains of the IGF-1 receptor. Two nearby residues, Asn 328 and Asn 337 are glycosylated. This

mutation is in a similar position to the insulin receptor mutant S323L which has aberrant insulin binding.

Several insertional mutants of the EGF receptor extracellular domain have been constructed to probe the role of several regions of the receptor (Harte, M.T. and Gentry, L.E., 1995, Arch. Biochem. Biophys. 322(2), 387-389). EGF receptor mutants with insertions at residues 162, 169, 174 and 220 bound EGF with a similar affinity to wild-type EGF receptor but bound TGF- α with a lower affinity than wild-type receptor. The first insertion was located in the region near the end of the L1 domain and the first cysteine of the first module in S1. The second and third insertions were present in the first module of S1 and the fourth insertion was present in the third module of S1. EGF receptor mutants with insertions at positions at 251 and 574 (both in large β -finger modules, the first in S1 and the second in S2) bound twice as much EGF as the wild type receptor. Two insertional mutants which showed reduced EGF receptor binding contained insertions at positions 291 and 474. The former insertion is contained in the seventh module of S1 which is a β -finger. The latter insertion is near the end of the L2 domain.

Another EGF receptor mutant which shows altered ligand binding behaviour is the R497K mutant. The site of this mutation in the first module of the S2 domain and faces the side of the L2 domain opposite to that containing residue 465. This mutant binds EGF in a similar fashion as wild-type receptor but abolishes the high affinity binding site for TGF- α (Moriai, T. et al, 1994, PNAS 91(21), 10217-10221).

It will be appreciated by persons skilled in the art that numerous variations and/or modifications may be made to the invention as shown in the specific embodiments without departing from the spirit or scope of the invention as broadly described. The present embodiments are, therefore, to be considered in all respects as illustrative and not restrictive.

Dated this twenty ninth day of May 1998

BIOMOLECULAR RESEARCH
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Patent Attorneys for the Applicant:

F B RICE & CO

Figure 1

IGF1R YVKIR-----
 IGF1R EICGPG--IDIRN-----DYQQLKRLN-CTVIEGYLHILLISK----AEDYRSY
 InsR lypgevc-pg--mdirn-----nltrlhelen-csvieghlqillmfk--trpedfrdl
 EGFR leekkv-c-qgtsnklqtglgtfedhflslqrmfnncevvlgnleityvqrny-----
 ErbB2 c-tgtdmklrlpaspethldmlrhlyqgcqvvggnleitylptna-----
 ErbB3 c-pgtlnglsvtgdangyqtlklyercevvmgnleivltghna-----
 ErbB4 c-agtenklsslsdleqqyral kyyencevmmgnleitsiehn-----

IGF1R ---HSHALVSLSFLKNLRLIL ILGEEQLEGNYSF
 IGF1R RFP-----KLTVITEYLLLFRVAGLESGLDLPNLTVIRGWKLFY-NYALVIF
 InsR sfp-----klimitdylllfrvygleslkdlfpnlvtirgsrlff-nyalvif
 EGFR -----dlsflkti qevagyvla-lntverip--lenlqiirgmmysyalavl
 ErbB2 -----slsflqdi qevagyvla-hnqvrqvp--lqrlrivrgtqlfednyalavl
 ErbB3 -----dlsflqw irevtgyvla-mnefstlp--lpnlrvvrgtqvvdgkfaifvm
 ErbB4 -----dlsflrsv revtgyvla-lnqfrylp--lenlriirgtklyedryalaif

IGF1R
 IGF1R EMT-----NLKDIGLYNLRNITRGAIRIEKNADLCYLSTVDWSLILD--A
 InsR emv-----hlkelglynlnm nitrsgvrieknnelcylatidwsrild--s
 EGR_19 snydankt-----glkelpmrnlqeilhgvrfssnpalcnvesiqwrdivssdf
 ErbB2 dngdplnnttpvtgaspgglrelqlrslteilkggvliqrnpqlcyqdtlwkdfhknn
 ErbB3 lnyntnssh-----alrqlrltqlteils ggyviekndklchmdtidwrdivrdrd
 ErbB4 lnyrkdgfn-----glqelglknlteilinggyvvdqnkflcyadti hwqdivrnpw

IGF1R CHPE-----CL-G-----SCSAPDNDTA---
 IGF1R VSNNYIV-GNK-PPKECGDLC---PGTMEEEKPMCE--KTTINNEYNYRCWT-----TNR
 InsR vednhiv-lnkddneecgdic---pgtakgktncp--atvingqfvercwt-----hsh
 EGFR lsnmsmdfqnh-lg-scq-kcdps-----cpng-----scwga-geen---
 ErbB2 qlaltlidtnr-sr-ach-pcspm-----ckgs-----rcwge-ssed---
 ErbB3 --aeivvkdng--r-scp-pchev-----ck-g-----rcwgp-gsed---
 ErbB4 psnltlvstng-ss-gcg-rchks-----ct-g-----rcwgp-tenh---
 1 1 1

IGF1R C CHPECLGS---CSAPDNDT---AC
 IGF1R CQ-----KMCPSTC---GKRACT-----ENNECCHPECLGSCSAPDNDTACVACRHYY
 InsR cq-----kvcptic---kshgct-----aeglcchseclgnscsqddptkcvacrnfy
 EGFR cqkltkii---caqqcsgr---crgk-sps---dcchnqcaagctgp-resdclvcrkfr
 ErbB2 cqsltrtv---caggca-r---ckgp-lpt---dccheqcaagctgp-khsdclaclhfn
 ErbB3 cqtltkti---capqcngh---cfgp-npn---qcchdecaggcsqp-qdtcdfacrhfn
 ErbB4 cqtltrtv---caeqcdgr---cygp-yvs---dcchrecaggcsqp-kdtcdfacmnfn
 1 2 2 2 23 3 3 3 4

IGF1R CVPA--CPPN-----
 IGF1R YAGVCVPACP-----PNTYRFEGWRCVDRDFC---ANILSAE---S
 InsR ldgrcvetcp-----ppyyhfqdwrcvnfsfc---qdlhhkcknsr
 EGFR deatckdtcpplmlynpttyqmdvnpegk---ysfg-atcvkk--cprn-----
 ErbB2 hsgicelhcpalvtyntdtfesmpnpegr---ytfg-ascvta--cpyn-----
 ErbB3 dsqacvprcpqplvynkltfqlepnphk---yqyg-gvcvas--cphn-----
 ErbB4 dsqacvtqcpqtfvynpttfqlehnfnak---ytyg-afcvkk--cphn-----
 4 5 5 6

IGF1R -----TYRFEGWRC
 IGF1R SDSEGFVIHD-GECEMCEPSGFIRNG-SQ-SMYCIPCEGPCPKV
 InsR rqqchqyvihnncipecpsgytmns-s--nllctpclgpcpkv
 EGFR -----yvvdthgscv racgadsyeme-edgvrkckkcegpckrv
 ErbB2 -----ylstdvgstlvcplhnqevtaedgtqrcekcskpcarv
 ErbB3 -----fvvdq-tscv racppdkmevd-knglkmcepcggclcpka
 ErbB4 -----fvvds-ssc vracpsskmeve-engikmckpctdicpka
 6 7 7 8 8

Figure 2

IGF1R
IGF1R EICGPGIDIRN-----DYQQLKRLNCTVIEGYLHILLIS-----
InsR lypgevc-pgmDIRN-----ltrlhelencsvieghlqillmf-----
EGFR c-ngigigefkdsIsinatnikhfkncTsisgdLhilpvafrgdsfthtppldp
ErbB2 c-yglgmehlrevravtsaniqefagckkifgslafpesfdgdpasntaplqp
ErbB3 c-egtgsgrfqt--vdssnidgfvnctkilgnldflitglnGdpwhkipaldp
ErbB4 c-dgigtgslmsaqtvdssnidkfinctkingnLiflvtgihgdpynaieaidp

IGF1R ILGEEQLEGN
IGF1R --KA--EDYRSYR-FPKLTVITEYLLLFRVA----GLES LGDLFPNLT VIRGWKLFY-N
InsR --ktrpedfrdls-fpklimitdylllfrvy----gleslkdLfpnlTVirgsrlff-n
EGFR qe-----ldilktvkeitgflliqawpenrtd----l-hafenleiirgrtkqhgg
ErbB2 eq-----lqvfetleeitgylyisawpdsldp----l-svfqnLqvirgrilhnGa
ErbB3 ek-----lnvfrtvreitgylniqswpphmhn----f-svfsnlTtiggrslynrg
ErbB4 ek-----lnvfrtvreitgflniqswppnmtd----f-svfsnlvtiggrvlys-g

IGF1R YSF
IGF1R YALVIFEMTNLKDIGLYNLRNITRGAIRIEKNADLCYLSTVDWSLILD--AVSN NYIVGN
InsR yalvifemvhlkelglynlmnitrgsvrieknnelcylatidwsrild--svednhivln
EGFR fslavvsl-nitslglrslkeisdgdviisgnknlcyantinwkkIfgt-sgqktkiIsn
ErbB2 ysltlqgl-giswlglrslrelgsglalihhnlhcfvhtvpwdqlfrn-phqallhtan
ErbB3 fsllimknlInvtslgfrslkeisagriyisanrqlcyhhslnwtkvLrgpteerldikhN
ErbB4 lslilkqq-gitslqfqsLkeisagniyitdnslncyhtinwttlfst-inqrivirdn

IGF1R CHPE-----CL-----GSCSAPDNDTA--CVACRHY
IGF1R K-PPKECGD---LC---PGTMEEKPMCEKTTINNEYNY--RCWT-----TNRC
InsR kddneecgd---ic---pgtakgktncpatvingqfve--rcwt-----hshc
EGFR r-gensckatgqvchal-----cs-----pegcwgp-eprd---cvscrnv
ErbB2 r-pedecvgeglachql-----ca-----rghcwgp-gptq---cvncsqf
ErbB3 r-prrdcvaegkvcdpl-----cs-----sggcwgp-gpgq---clscrnY
ErbB4 r-kaenctaegmvcnhl-----cs-----sdgcwgp-gpdq---clscrff
1 1 1 1 2

IGF1R YYAGVCVPACPPNTYRF-----EGW-----RC CHPECLG-----SCSAPDNDTAC
IGF1R CPSGFIRN-----GSQSMYCIPCEG
EGFR srgrecvdckkllegeprefvens-----eci qchpeclpqa-mnitctgr-gpdnc
ErbB2 lrgqecveecrvlqglpreyvnaR-----hclpchpecqpqn-gsvtcfgp-eadqc
ErbB3 srggvcvthcnflngeprefahea-----ecfschpecqpme-gtatcnGs-gsdTc
ErbB4 srgriciescnlydgefrefengs-----icvecdpqcekmedglltchgp-gpdnc
2 3 3 4 4 4 4

IGF1R VACRHYYYAGVCVPACPPNTYRF-----EGW-----RC CHPECLGSCSA
IGF1R CPSGFIRN-----GSQSMYCIPCEG
EGFR iqcahyidgphcvktcpagvmgenntl-vwkyadagh-----vchlchpncTygctg
ErbB2 vacahykdppfcvarcpsgvkpdlsympiwkfpdeeg-----acqpcpincthscvd
ErbB3 aqcahfrdgphcvsscphgvlgak--gpiykypdvqn-----ecrpchenctqgckg
ErbB4 tkcshfkdgpnCvekcpgdglqgan--sfifkyadpdr-----echpchnctqgcng
5 5 6 6 7 7 7

IGF1R PDNDTAC
IGF1R
EGFR p-glegcptngpkips
ErbB2 l-ddkgc
ErbB3 p-elqdc
ErbB4 p-tshdc
7

Figure 3



Figure 4

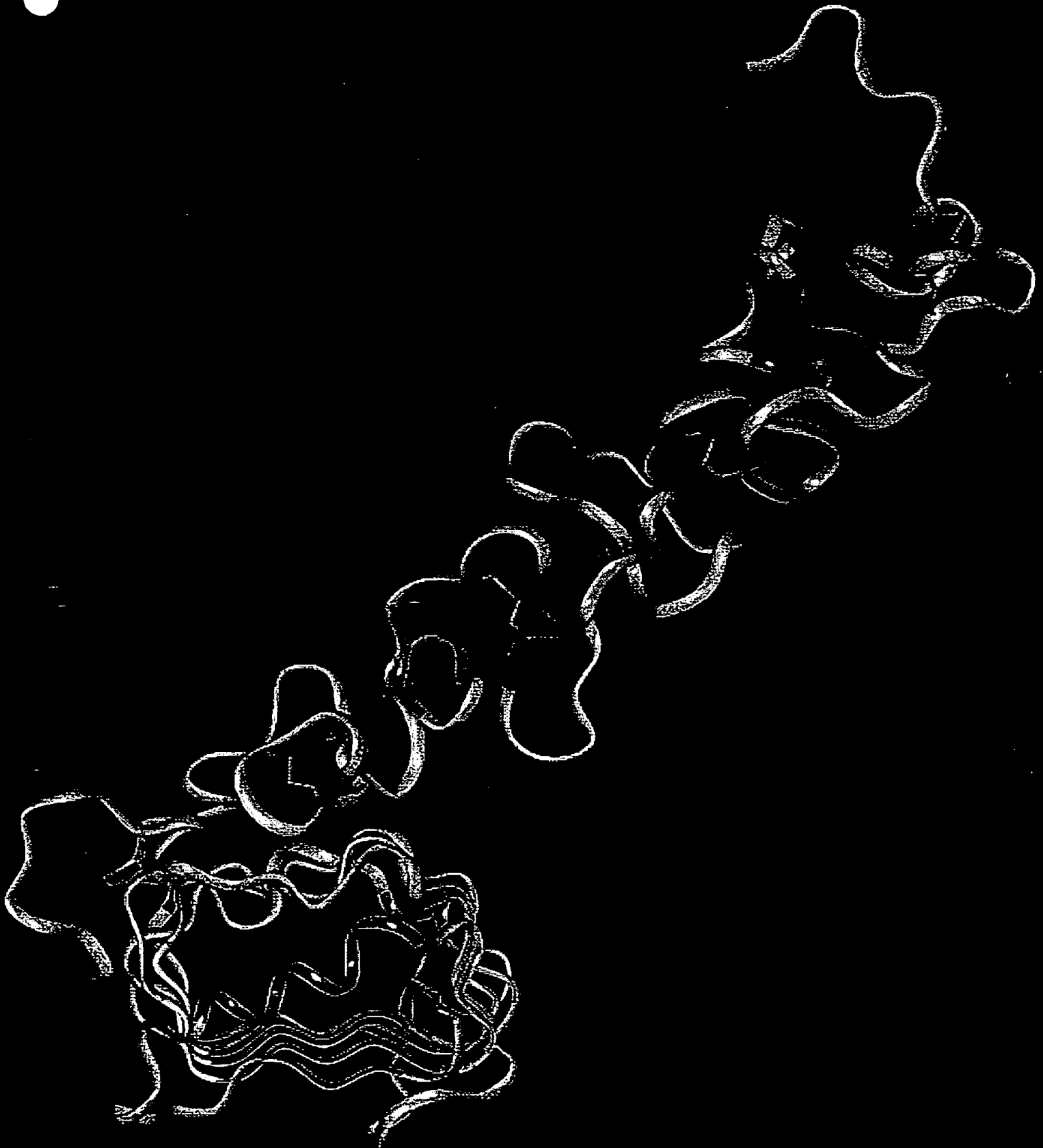
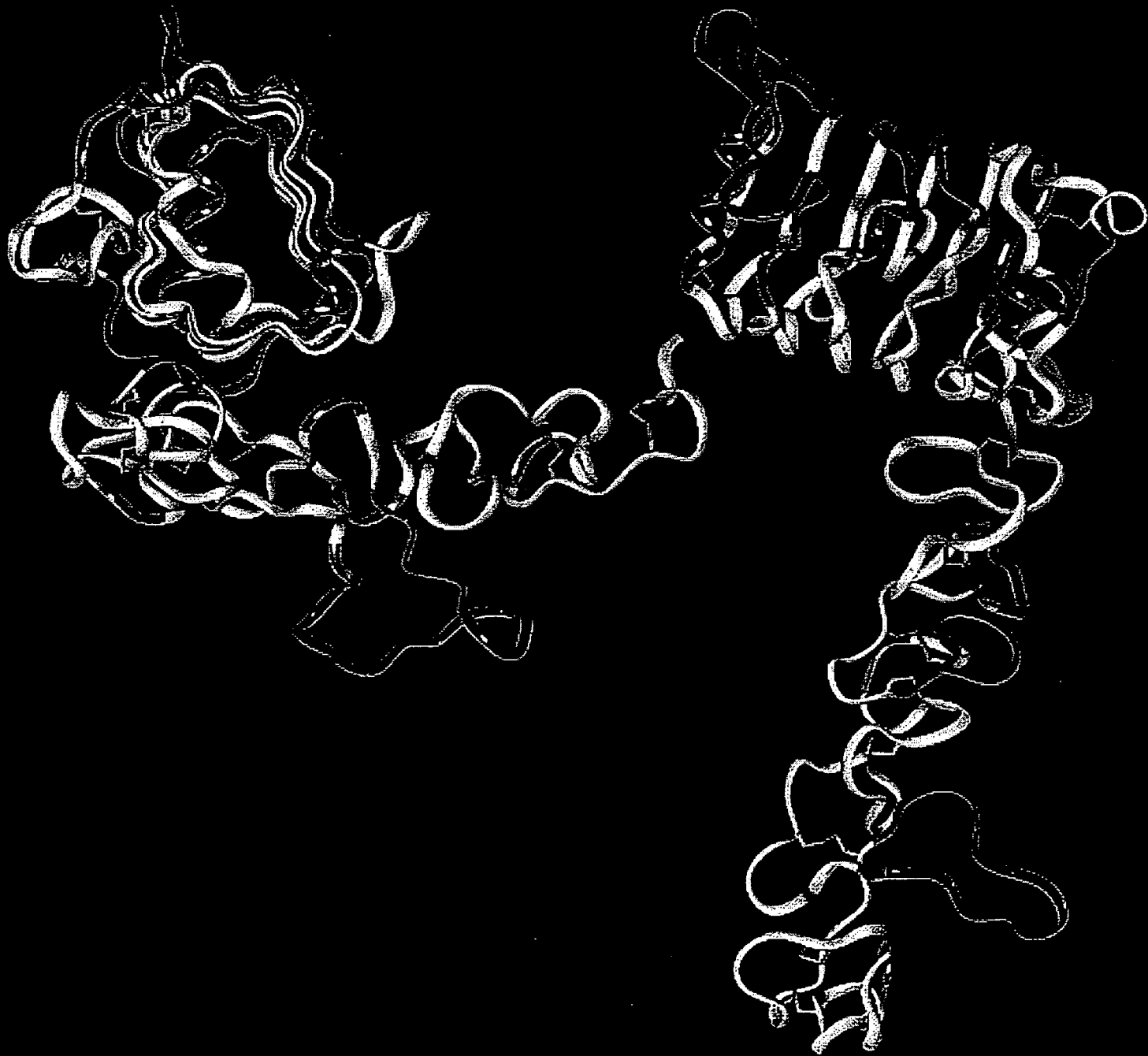


Figure 5



| | | | | | | | | | |
|------|----|-----|-----|---|--------|--------|--------|------|-------|
| ATOM | 3 | N | LEU | 1 | 60.296 | 19.487 | 71.703 | 1.00 | 60.00 |
| ATOM | 5 | CA | LEU | 1 | 59.489 | 18.323 | 71.270 | 1.00 | 60.00 |
| ATOM | 6 | CB | LEU | 1 | 59.216 | 18.373 | 69.755 | 1.00 | 60.00 |
| ATOM | 7 | CG | LEU | 1 | 58.289 | 19.520 | 69.302 | 1.00 | 60.00 |
| ATOM | 8 | CD1 | LEU | 1 | 56.879 | 19.357 | 69.888 | 1.00 | 60.00 |
| ATOM | 9 | CD2 | LEU | 1 | 58.903 | 20.902 | 69.580 | 1.00 | 60.00 |
| ATOM | 10 | C | LEU | 1 | 60.208 | 17.051 | 71.563 | 1.00 | 60.00 |
| ATOM | 11 | O | LEU | 1 | 61.087 | 16.999 | 72.421 | 1.00 | 60.00 |
| ATOM | 12 | N | GLU | 2 | 59.824 | 15.976 | 70.853 | 1.00 | 60.00 |
| ATOM | 14 | CA | GLU | 2 | 60.463 | 14.712 | 71.045 | 1.00 | 60.00 |
| ATOM | 15 | CB | GLU | 2 | 59.551 | 13.646 | 71.675 | 1.00 | 60.00 |
| ATOM | 16 | CG | GLU | 2 | 59.244 | 13.895 | 73.153 | 1.00 | 60.00 |
| ATOM | 17 | CD | GLU | 2 | 60.480 | 13.515 | 73.955 | 1.00 | 60.00 |
| ATOM | 18 | OE1 | GLU | 2 | 60.436 | 13.645 | 75.208 | 1.00 | 60.00 |
| ATOM | 19 | OE2 | GLU | 2 | 61.485 | 13.084 | 73.327 | 1.00 | 60.00 |
| ATOM | 20 | C | GLU | 2 | 60.842 | 14.217 | 69.692 | 1.00 | 60.00 |
| ATOM | 21 | O | GLU | 2 | 60.830 | 14.962 | 68.714 | 1.00 | 60.00 |
| ATOM | 22 | N | GLU | 3 | 61.212 | 12.928 | 69.615 | 1.00 | 60.00 |
| ATOM | 24 | CA | GLU | 3 | 61.583 | 12.345 | 68.364 | 1.00 | 60.00 |
| ATOM | 25 | CB | GLU | 3 | 62.012 | 10.876 | 68.513 | 1.00 | 60.00 |
| ATOM | 26 | CG | GLU | 3 | 60.926 | 9.981 | 69.116 | 1.00 | 60.00 |
| ATOM | 27 | CD | GLU | 3 | 61.538 | 8.616 | 69.395 | 1.00 | 60.00 |
| ATOM | 28 | OE1 | GLU | 3 | 62.780 | 8.481 | 69.232 | 1.00 | 60.00 |
| ATOM | 29 | OE2 | GLU | 3 | 60.774 | 7.691 | 69.781 | 1.00 | 60.00 |
| ATOM | 30 | C | GLU | 3 | 60.382 | 12.401 | 67.479 | 1.00 | 60.00 |
| ATOM | 31 | O | GLU | 3 | 60.473 | 12.789 | 66.316 | 1.00 | 60.00 |
| ATOM | 32 | N | LYS | 4 | 59.209 | 12.029 | 68.025 | 1.00 | 60.00 |
| ATOM | 34 | CA | LYS | 4 | 58.014 | 12.055 | 67.238 | 1.00 | 60.00 |
| ATOM | 35 | CB | LYS | 4 | 56.883 | 11.191 | 67.818 | 1.00 | 60.00 |
| ATOM | 36 | CG | LYS | 4 | 55.752 | 10.920 | 66.828 | 1.00 | 60.00 |
| ATOM | 37 | CD | LYS | 4 | 56.125 | 9.887 | 65.766 | 1.00 | 60.00 |
| ATOM | 38 | CE | LYS | 4 | 56.026 | 8.449 | 66.279 | 1.00 | 60.00 |
| ATOM | 39 | NZ | LYS | 4 | 56.881 | 8.282 | 67.477 | 1.00 | 60.00 |
| ATOM | 43 | C | LYS | 4 | 57.530 | 13.466 | 67.246 | 1.00 | 60.00 |
| ATOM | 44 | O | LYS | 4 | 57.866 | 14.236 | 68.144 | 1.00 | 60.00 |
| ATOM | 45 | N | LYS | 5 | 56.738 | 13.855 | 66.229 | 1.00 | 40.00 |
| ATOM | 47 | CA | LYS | 5 | 56.253 | 15.201 | 66.238 | 1.00 | 40.00 |
| ATOM | 48 | CB | LYS | 5 | 57.260 | 16.226 | 65.673 | 1.00 | 40.00 |
| ATOM | 49 | CG | LYS | 5 | 56.923 | 17.682 | 66.018 | 1.00 | 40.00 |
| ATOM | 50 | CD | LYS | 5 | 58.055 | 18.677 | 65.752 | 1.00 | 40.00 |
| ATOM | 51 | CE | LYS | 5 | 57.687 | 20.121 | 66.109 | 1.00 | 40.00 |
| ATOM | 52 | NZ | LYS | 5 | 58.848 | 21.016 | 65.897 | 1.00 | 40.00 |
| ATOM | 56 | C | LYS | 5 | 55.006 | 15.267 | 65.418 | 1.00 | 40.00 |
| ATOM | 57 | O | LYS | 5 | 54.478 | 14.249 | 64.973 | 1.00 | 40.00 |
| ATOM | 58 | N | VAL | 6 | 54.492 | 16.496 | 65.229 | 1.00 | 40.00 |
| ATOM | 60 | CA | VAL | 6 | 53.310 | 16.742 | 64.461 | 1.00 | 40.00 |
| ATOM | 61 | CB | VAL | 6 | 52.718 | 18.092 | 64.761 | 1.00 | 40.00 |
| ATOM | 62 | CG1 | VAL | 6 | 51.500 | 18.346 | 63.858 | 1.00 | 40.00 |
| ATOM | 63 | CG2 | VAL | 6 | 52.397 | 18.149 | 66.263 | 1.00 | 40.00 |
| ATOM | 64 | C | VAL | 6 | 53.718 | 16.713 | 63.024 | 1.00 | 40.00 |
| ATOM | 65 | O | VAL | 6 | 54.901 | 16.835 | 62.709 | 1.00 | 40.00 |
| ATOM | 66 | N | CYS | 7 | 52.749 | 16.513 | 62.107 | 1.00 | 40.00 |
| ATOM | 68 | CA | CYS | 7 | 53.077 | 16.507 | 60.711 | 1.00 | 40.00 |
| ATOM | 69 | CB | CYS | 7 | 53.033 | 15.116 | 60.050 | 1.00 | 40.00 |
| ATOM | 70 | SG | CYS | 7 | 51.430 | 14.278 | 60.192 | 1.00 | 40.00 |
| ATOM | 71 | C | CYS | 7 | 52.115 | 17.399 | 59.995 | 1.00 | 40.00 |
| ATOM | 72 | O | CYS | 7 | 51.133 | 17.864 | 60.567 | 1.00 | 40.00 |
| ATOM | 73 | N | GLN | 8 | 52.398 | 17.681 | 58.711 | 1.00 | 40.00 |
| ATOM | 75 | CA | GLN | 8 | 51.565 | 18.559 | 57.947 | 1.00 | 40.00 |
| ATOM | 76 | CB | GLN | 8 | 52.249 | 19.057 | 56.664 | 1.00 | 40.00 |
| ATOM | 77 | CG | GLN | 8 | 52.592 | 17.934 | 55.683 | 1.00 | 40.00 |
| ATOM | 78 | CD | GLN | 8 | 53.346 | 18.542 | 54.510 | 1.00 | 40.00 |
| ATOM | 79 | OE1 | GLN | 8 | 54.534 | 18.846 | 54.609 | 1.00 | 40.00 |
| ATOM | 80 | NE2 | GLN | 8 | 52.638 | 18.727 | 53.364 | 1.00 | 40.00 |

Figure 6

| | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 83 | C | GLN | 8 | 50.310 | 17.853 | 57.564 | 1.00 | 40.00 |
| ATOM | 84 | O | GLN | 8 | 50.163 | 16.646 | 57.754 | 1.00 | 40.00 |
| ATOM | 85 | N | GLY | 9 | 49.354 | 18.626 | 57.021 | 1.00 | 40.00 |
| ATOM | 87 | CA | GLY | 9 | 48.094 | 18.108 | 56.597 | 1.00 | 40.00 |
| ATOM | 88 | C | GLY | 9 | 47.630 | 19.103 | 55.597 | 1.00 | 40.00 |
| ATOM | 89 | O | GLY | 9 | 46.441 | 19.207 | 55.311 | 1.00 | 40.00 |
| ATOM | 90 | N | THR | 10 | 48.583 | 19.883 | 55.052 | 1.00 | 40.00 |
| ATOM | 92 | CA | THR | 10 | 48.228 | 20.808 | 54.023 | 1.00 | 40.00 |
| ATOM | 93 | CB | THR | 10 | 49.373 | 21.659 | 53.561 | 1.00 | 40.00 |
| ATOM | 94 | OG1 | THR | 10 | 49.884 | 22.424 | 54.644 | 1.00 | 40.00 |
| ATOM | 96 | CG2 | THR | 10 | 48.875 | 22.586 | 52.440 | 1.00 | 40.00 |
| ATOM | 97 | C | THR | 10 | 47.861 | 19.897 | 52.908 | 1.00 | 40.00 |
| ATOM | 98 | O | THR | 10 | 48.727 | 19.416 | 52.179 | 1.00 | 40.00 |
| ATOM | 99 | N | SER | 11 | 46.547 | 19.653 | 52.754 | 1.00 | 40.00 |
| ATOM | 101 | CA | SER | 11 | 46.075 | 18.684 | 51.822 | 1.00 | 40.00 |
| ATOM | 102 | CB | SER | 11 | 46.297 | 19.088 | 50.356 | 1.00 | 40.00 |
| ATOM | 103 | OG | SER | 11 | 45.542 | 20.251 | 50.051 | 1.00 | 40.00 |
| ATOM | 105 | C | SER | 11 | 46.842 | 17.433 | 52.099 | 1.00 | 40.00 |
| ATOM | 106 | O | SER | 11 | 47.460 | 16.877 | 51.193 | 1.00 | 40.00 |
| ATOM | 107 | N | ASN | 12 | 46.840 | 16.960 | 53.368 | 1.00 | 40.00 |
| ATOM | 109 | CA | ASN | 12 | 47.566 | 15.750 | 53.624 | 1.00 | 40.00 |
| ATOM | 110 | CB | ASN | 12 | 47.743 | 15.405 | 55.113 | 1.00 | 40.00 |
| ATOM | 111 | CG | ASN | 12 | 48.722 | 14.241 | 55.199 | 1.00 | 40.00 |
| ATOM | 112 | OD1 | ASN | 12 | 49.066 | 13.628 | 54.189 | 1.00 | 40.00 |
| ATOM | 113 | ND2 | ASN | 12 | 49.182 | 13.922 | 56.438 | 1.00 | 40.00 |
| ATOM | 116 | C | ASN | 12 | 46.715 | 14.696 | 53.020 | 1.00 | 40.00 |
| ATOM | 117 | O | ASN | 12 | 45.802 | 14.172 | 53.657 | 1.00 | 40.00 |
| ATOM | 118 | N | LYS | 13 | 46.993 | 14.364 | 51.749 | 1.00 | 40.00 |
| ATOM | 120 | CA | LYS | 13 | 46.144 | 13.421 | 51.104 | 1.00 | 40.00 |
| ATOM | 121 | CB | LYS | 13 | 45.416 | 14.008 | 49.884 | 1.00 | 40.00 |
| ATOM | 122 | CG | LYS | 13 | 46.363 | 14.573 | 48.825 | 1.00 | 40.00 |
| ATOM | 123 | CD | LYS | 13 | 45.675 | 14.921 | 47.505 | 1.00 | 40.00 |
| ATOM | 124 | CE | LYS | 13 | 46.617 | 15.551 | 46.477 | 1.00 | 40.00 |
| ATOM | 125 | NZ | LYS | 13 | 45.877 | 15.863 | 45.233 | 1.00 | 40.00 |
| ATOM | 129 | C | LYS | 13 | 46.913 | 12.234 | 50.648 | 1.00 | 40.00 |
| ATOM | 130 | O | LYS | 13 | 47.735 | 12.310 | 49.737 | 1.00 | 40.00 |
| ATOM | 131 | N | LEU | 14 | 46.652 | 11.096 | 51.310 | 1.00 | 40.00 |
| ATOM | 133 | CA | LEU | 14 | 47.211 | 9.852 | 50.895 | 1.00 | 40.00 |
| ATOM | 134 | CB | LEU | 14 | 46.976 | 8.748 | 51.947 | 1.00 | 40.00 |
| ATOM | 135 | CG | LEU | 14 | 47.540 | 7.360 | 51.598 | 1.00 | 40.00 |
| ATOM | 136 | CD1 | LEU | 14 | 46.871 | 6.739 | 50.371 | 1.00 | 40.00 |
| ATOM | 137 | CD2 | LEU | 14 | 49.076 | 7.413 | 51.504 | 1.00 | 40.00 |
| ATOM | 138 | C | LEU | 14 | 46.341 | 9.560 | 49.715 | 1.00 | 40.00 |
| ATOM | 139 | O | LEU | 14 | 45.124 | 9.706 | 49.797 | 1.00 | 40.00 |
| ATOM | 140 | N | THR | 15 | 46.926 | 9.175 | 48.565 | 1.00 | 20.00 |
| ATOM | 142 | CA | THR | 15 | 46.046 | 8.932 | 47.460 | 1.00 | 20.00 |
| ATOM | 143 | CB | THR | 15 | 45.720 | 10.173 | 46.680 | 1.00 | 20.00 |
| ATOM | 144 | OG1 | THR | 15 | 44.734 | 9.894 | 45.699 | 1.00 | 20.00 |
| ATOM | 146 | CG2 | THR | 15 | 47.008 | 10.693 | 46.016 | 1.00 | 20.00 |
| ATOM | 147 | C | THR | 15 | 46.662 | 7.957 | 46.516 | 1.00 | 20.00 |
| ATOM | 148 | O | THR | 15 | 47.882 | 7.845 | 46.427 | 1.00 | 20.00 |
| ATOM | 149 | N | GLN | 16 | 45.812 | 7.213 | 45.784 | 1.00 | 20.00 |
| ATOM | 151 | CA | GLN | 16 | 46.308 | 6.267 | 44.830 | 1.00 | 20.00 |
| ATOM | 152 | CB | GLN | 16 | 45.194 | 5.417 | 44.193 | 1.00 | 20.00 |
| ATOM | 153 | CG | GLN | 16 | 45.677 | 4.384 | 43.166 | 1.00 | 20.00 |
| ATOM | 154 | CD | GLN | 16 | 45.903 | 5.076 | 41.826 | 1.00 | 20.00 |
| ATOM | 155 | OE1 | GLN | 16 | 46.999 | 5.031 | 41.269 | 1.00 | 20.00 |
| ATOM | 156 | NE2 | GLN | 16 | 44.838 | 5.737 | 41.296 | 1.00 | 20.00 |
| ATOM | 159 | C | GLN | 16 | 46.943 | 7.055 | 43.737 | 1.00 | 20.00 |
| ATOM | 160 | O | GLN | 16 | 48.054 | 6.749 | 43.312 | 1.00 | 20.00 |
| ATOM | 161 | N | LEU | 17 | 46.237 | 8.105 | 43.275 | 1.00 | 20.00 |
| ATOM | 163 | CA | LEU | 17 | 46.700 | 8.915 | 42.189 | 1.00 | 20.00 |
| ATOM | 164 | CB | LEU | 17 | 45.794 | 10.142 | 41.941 | 1.00 | 20.00 |
| ATOM | 165 | CG | LEU | 17 | 46.211 | 11.086 | 40.792 | 1.00 | 20.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 166 | CD1 | LEU | 17 | 47.470 | 11.904 | 41.126 | 1.00 | 20.00 |
| ATOM | 167 | CD2 | LEU | 17 | 46.324 | 10.326 | 39.462 | 1.00 | 20.00 |
| ATOM | 168 | C | LEU | 17 | 48.081 | 9.372 | 42.501 | 1.00 | 20.00 |
| ATOM | 169 | O | LEU | 17 | 48.436 | 9.591 | 43.657 | 1.00 | 20.00 |
| ATOM | 170 | N | GLY | 18 | 48.912 | 9.499 | 41.455 | 1.00 | 20.00 |
| ATOM | 172 | CA | GLY | 18 | 50.262 | 9.939 | 41.643 | 1.00 | 20.00 |
| ATOM | 173 | C | GLY | 18 | 51.057 | 9.374 | 40.516 | 1.00 | 20.00 |
| ATOM | 174 | O | GLY | 18 | 50.876 | 8.222 | 40.127 | 1.00 | 20.00 |
| ATOM | 175 | N | THR | 19 | 51.972 | 10.189 | 39.961 | 1.00 | 20.00 |
| ATOM | 177 | CA | THR | 19 | 52.782 | 9.709 | 38.886 | 1.00 | 20.00 |
| ATOM | 178 | CB | THR | 19 | 53.666 | 10.769 | 38.292 | 1.00 | 20.00 |
| ATOM | 179 | OG1 | THR | 19 | 54.347 | 10.254 | 37.158 | 1.00 | 20.00 |
| ATOM | 181 | CG2 | THR | 19 | 54.670 | 11.258 | 39.347 | 1.00 | 20.00 |
| ATOM | 182 | C | THR | 19 | 53.635 | 8.619 | 39.436 | 1.00 | 20.00 |
| ATOM | 183 | O | THR | 19 | 53.833 | 7.588 | 38.796 | 1.00 | 20.00 |
| ATOM | 184 | N | PHE | 20 | 54.148 | 8.817 | 40.664 | 1.00 | 20.00 |
| ATOM | 186 | CA | PHE | 20 | 54.987 | 7.834 | 41.278 | 1.00 | 20.00 |
| ATOM | 187 | CB | PHE | 20 | 55.635 | 8.347 | 42.579 | 1.00 | 20.00 |
| ATOM | 188 | CG | PHE | 20 | 56.659 | 7.367 | 43.040 | 1.00 | 20.00 |
| ATOM | 189 | CD1 | PHE | 20 | 57.923 | 7.381 | 42.496 | 1.00 | 20.00 |
| ATOM | 190 | CD2 | PHE | 20 | 56.398 | 6.515 | 44.089 | 1.00 | 20.00 |
| ATOM | 191 | CE1 | PHE | 20 | 58.900 | 6.537 | 42.967 | 1.00 | 20.00 |
| ATOM | 192 | CE2 | PHE | 20 | 57.373 | 5.673 | 44.569 | 1.00 | 20.00 |
| ATOM | 193 | CZ | PHE | 20 | 58.627 | 5.682 | 44.007 | 1.00 | 20.00 |
| ATOM | 194 | C | PHE | 20 | 54.090 | 6.693 | 41.619 | 1.00 | 20.00 |
| ATOM | 195 | O | PHE | 20 | 52.871 | 6.793 | 41.490 | 1.00 | 20.00 |
| ATOM | 196 | N | GLU | 21 | 54.671 | 5.558 | 42.047 | 1.00 | 20.00 |
| ATOM | 198 | CA | GLU | 21 | 53.833 | 4.450 | 42.396 | 1.00 | 20.00 |
| ATOM | 199 | CB | GLU | 21 | 54.593 | 3.121 | 42.541 | 1.00 | 20.00 |
| ATOM | 200 | CG | GLU | 21 | 55.122 | 2.564 | 41.219 | 1.00 | 20.00 |
| ATOM | 201 | CD | GLU | 21 | 55.844 | 1.259 | 41.522 | 1.00 | 20.00 |
| ATOM | 202 | OE1 | GLU | 21 | 56.277 | 0.584 | 40.550 | 1.00 | 20.00 |
| ATOM | 203 | OE2 | GLU | 21 | 55.970 | 0.918 | 42.729 | 1.00 | 20.00 |
| ATOM | 204 | C | GLU | 21 | 53.254 | 4.782 | 43.725 | 1.00 | 20.00 |
| ATOM | 205 | O | GLU | 21 | 53.828 | 4.458 | 44.764 | 1.00 | 20.00 |
| ATOM | 206 | N | ASP | 22 | 52.087 | 5.454 | 43.721 | 1.00 | 20.00 |
| ATOM | 208 | CA | ASP | 22 | 51.483 | 5.831 | 44.961 | 1.00 | 20.00 |
| ATOM | 209 | CB | ASP | 22 | 50.885 | 7.248 | 44.940 | 1.00 | 20.00 |
| ATOM | 210 | CG | ASP | 22 | 50.624 | 7.676 | 46.376 | 1.00 | 20.00 |
| ATOM | 211 | OD1 | ASP | 22 | 50.950 | 8.847 | 46.707 | 1.00 | 20.00 |
| ATOM | 212 | OD2 | ASP | 22 | 50.091 | 6.845 | 47.159 | 1.00 | 20.00 |
| ATOM | 213 | C | ASP | 22 | 50.379 | 4.864 | 45.231 | 1.00 | 20.00 |
| ATOM | 214 | O | ASP | 22 | 49.567 | 4.565 | 44.357 | 1.00 | 20.00 |
| ATOM | 215 | N | HIS | 23 | 50.341 | 4.335 | 46.467 | 1.00 | 40.00 |
| ATOM | 217 | CA | HIS | 23 | 49.347 | 3.384 | 46.853 | 1.00 | 40.00 |
| ATOM | 218 | CB | HIS | 23 | 49.761 | 1.915 | 46.649 | 1.00 | 40.00 |
| ATOM | 219 | CG | HIS | 23 | 49.838 | 1.473 | 45.220 | 1.00 | 40.00 |
| ATOM | 220 | CD2 | HIS | 23 | 50.917 | 1.323 | 44.403 | 1.00 | 40.00 |
| ATOM | 221 | ND1 | HIS | 23 | 48.750 | 1.052 | 44.486 | 1.00 | 40.00 |
| ATOM | 223 | CE1 | HIS | 23 | 49.222 | 0.673 | 43.271 | 1.00 | 40.00 |
| ATOM | 224 | NE2 | HIS | 23 | 50.530 | 0.820 | 43.174 | 1.00 | 40.00 |
| ATOM | 226 | C | HIS | 23 | 49.165 | 3.538 | 48.323 | 1.00 | 40.00 |
| ATOM | 227 | O | HIS | 23 | 49.412 | 4.596 | 48.899 | 1.00 | 40.00 |
| ATOM | 228 | N | PHE | 24 | 48.700 | 2.447 | 48.952 | 1.00 | 40.00 |
| ATOM | 230 | CA | PHE | 24 | 48.497 | 2.366 | 50.365 | 1.00 | 40.00 |
| ATOM | 231 | CB | PHE | 24 | 47.878 | 1.032 | 50.798 | 1.00 | 40.00 |
| ATOM | 232 | CG | PHE | 24 | 47.619 | 1.074 | 52.265 | 1.00 | 40.00 |
| ATOM | 233 | CD1 | PHE | 24 | 46.418 | 1.545 | 52.742 | 1.00 | 40.00 |
| ATOM | 234 | CD2 | PHE | 24 | 48.565 | 0.632 | 53.162 | 1.00 | 40.00 |
| ATOM | 235 | CE1 | PHE | 24 | 46.157 | 1.564 | 54.092 | 1.00 | 40.00 |
| ATOM | 236 | CE2 | PHE | 24 | 48.312 | 0.655 | 54.513 | 1.00 | 40.00 |
| ATOM | 237 | CZ | PHE | 24 | 47.105 | 1.118 | 54.981 | 1.00 | 40.00 |
| ATOM | 238 | C | PHE | 24 | 49.858 | 2.476 | 50.972 | 1.00 | 40.00 |
| ATOM | 239 | O | PHE | 24 | 50.016 | 2.876 | 52.124 | 1.00 | 40.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 554 | C | LEU | 55 | 48.807 | 3.909 | 63.695 | 1.00 | 40.00 |
| ATOM | 555 | O | LEU | 55 | 47.740 | 4.362 | 64.108 | 1.00 | 40.00 |
| ATOM | 556 | N | LYS | 56 | 49.696 | 3.297 | 64.498 | 1.00 | 40.00 |
| ATOM | 558 | CA | LYS | 56 | 49.497 | 3.101 | 65.901 | 1.00 | 40.00 |
| ATOM | 559 | CB | LYS | 56 | 50.576 | 2.185 | 66.506 | 1.00 | 40.00 |
| ATOM | 560 | CG | LYS | 56 | 50.417 | 1.939 | 68.008 | 1.00 | 40.00 |
| ATOM | 561 | CD | LYS | 56 | 51.365 | 0.867 | 68.554 | 1.00 | 40.00 |
| ATOM | 562 | CE | LYS | 56 | 52.806 | 1.355 | 68.725 | 1.00 | 40.00 |
| ATOM | 563 | NZ | LYS | 56 | 53.656 | 0.266 | 69.255 | 1.00 | 40.00 |
| ATOM | 567 | C | LYS | 56 | 49.574 | 4.403 | 66.636 | 1.00 | 40.00 |
| ATOM | 568 | O | LYS | 56 | 48.753 | 4.684 | 67.506 | 1.00 | 40.00 |
| ATOM | 569 | N | THR | 57 | 50.566 | 5.235 | 66.273 | 1.00 | 20.00 |
| ATOM | 571 | CA | THR | 57 | 50.892 | 6.456 | 66.958 | 1.00 | 20.00 |
| ATOM | 572 | CB | THR | 57 | 52.151 | 7.079 | 66.433 | 1.00 | 20.00 |
| ATOM | 573 | OG1 | THR | 57 | 52.558 | 8.147 | 67.275 | 1.00 | 20.00 |
| ATOM | 575 | CG2 | THR | 57 | 51.890 | 7.590 | 65.006 | 1.00 | 20.00 |
| ATOM | 576 | C | THR | 57 | 49.837 | 7.520 | 66.919 | 1.00 | 20.00 |
| ATOM | 577 | O | THR | 57 | 49.634 | 8.217 | 67.911 | 1.00 | 20.00 |
| ATOM | 578 | N | ILE | 58 | 49.134 | 7.669 | 65.781 | 1.00 | 20.00 |
| ATOM | 580 | CA | ILE | 58 | 48.202 | 8.749 | 65.585 | 1.00 | 20.00 |
| ATOM | 581 | CB | ILE | 58 | 47.381 | 8.578 | 64.339 | 1.00 | 20.00 |
| ATOM | 582 | CG2 | ILE | 58 | 46.356 | 9.724 | 64.289 | 1.00 | 20.00 |
| ATOM | 583 | CG1 | ILE | 58 | 48.286 | 8.508 | 63.097 | 1.00 | 20.00 |
| ATOM | 584 | CD1 | ILE | 58 | 49.117 | 9.770 | 62.877 | 1.00 | 20.00 |
| ATOM | 585 | C | ILE | 58 | 47.233 | 8.931 | 66.716 | 1.00 | 20.00 |
| ATOM | 586 | O | ILE | 58 | 46.204 | 8.260 | 66.774 | 1.00 | 20.00 |
| ATOM | 587 | N | GLN | 59 | 47.579 | 9.822 | 67.672 | 1.00 | 20.00 |
| ATOM | 589 | CA | GLN | 59 | 46.734 | 10.199 | 68.773 | 1.00 | 20.00 |
| ATOM | 590 | CB | GLN | 59 | 47.517 | 10.863 | 69.915 | 1.00 | 20.00 |
| ATOM | 591 | CG | GLN | 59 | 48.143 | 12.195 | 69.501 | 1.00 | 20.00 |
| ATOM | 592 | CD | GLN | 59 | 48.757 | 12.832 | 70.736 | 1.00 | 20.00 |
| ATOM | 593 | OE1 | GLN | 59 | 49.685 | 12.297 | 71.340 | 1.00 | 20.00 |
| ATOM | 594 | NE2 | GLN | 59 | 48.215 | 14.014 | 71.129 | 1.00 | 20.00 |
| ATOM | 597 | C | GLN | 59 | 45.679 | 11.189 | 68.377 | 1.00 | 20.00 |
| ATOM | 598 | O | GLN | 59 | 44.530 | 11.095 | 68.808 | 1.00 | 20.00 |
| ATOM | 599 | N | GLU | 60 | 46.048 | 12.190 | 67.550 | 1.00 | 20.00 |
| ATOM | 601 | CA | GLU | 60 | 45.095 | 13.224 | 67.262 | 1.00 | 20.00 |
| ATOM | 602 | CB | GLU | 60 | 45.290 | 14.461 | 68.155 | 1.00 | 20.00 |
| ATOM | 603 | CG | GLU | 60 | 44.250 | 15.563 | 67.946 | 1.00 | 20.00 |
| ATOM | 604 | CD | GLU | 60 | 44.647 | 16.742 | 68.822 | 1.00 | 20.00 |
| ATOM | 605 | OE1 | GLU | 60 | 43.756 | 17.283 | 69.530 | 1.00 | 20.00 |
| ATOM | 606 | OE2 | GLU | 60 | 45.848 | 17.123 | 68.787 | 1.00 | 20.00 |
| ATOM | 607 | C | GLU | 60 | 45.206 | 13.695 | 65.848 | 1.00 | 20.00 |
| ATOM | 608 | O | GLU | 60 | 46.181 | 13.420 | 65.153 | 1.00 | 20.00 |
| ATOM | 609 | N | VAL | 61 | 44.145 | 14.383 | 65.381 | 1.00 | 20.00 |
| ATOM | 611 | CA | VAL | 61 | 44.109 | 15.031 | 64.104 | 1.00 | 20.00 |
| ATOM | 612 | CB | VAL | 61 | 43.283 | 14.315 | 63.069 | 1.00 | 20.00 |
| ATOM | 613 | CG1 | VAL | 61 | 41.843 | 14.146 | 63.582 | 1.00 | 20.00 |
| ATOM | 614 | CG2 | VAL | 61 | 43.376 | 15.105 | 61.752 | 1.00 | 20.00 |
| ATOM | 615 | C | VAL | 61 | 43.469 | 16.347 | 64.419 | 1.00 | 20.00 |
| ATOM | 616 | O | VAL | 61 | 42.399 | 16.407 | 65.018 | 1.00 | 20.00 |
| ATOM | 617 | N | ALA | 62 | 44.133 | 17.447 | 64.037 | 1.00 | 20.00 |
| ATOM | 619 | CA | ALA | 62 | 43.683 | 18.774 | 64.335 | 1.00 | 20.00 |
| ATOM | 620 | CB | ALA | 62 | 44.789 | 19.827 | 64.147 | 1.00 | 20.00 |
| ATOM | 621 | C | ALA | 62 | 42.528 | 19.201 | 63.488 | 1.00 | 20.00 |
| ATOM | 622 | O | ALA | 62 | 42.002 | 20.294 | 63.685 | 1.00 | 20.00 |
| ATOM | 623 | N | GLY | 63 | 42.161 | 18.409 | 62.461 | 1.00 | 20.00 |
| ATOM | 625 | CA | GLY | 63 | 41.087 | 18.809 | 61.595 | 1.00 | 20.00 |
| ATOM | 626 | C | GLY | 63 | 40.025 | 17.758 | 61.501 | 1.00 | 20.00 |
| ATOM | 627 | O | GLY | 63 | 39.332 | 17.458 | 62.470 | 1.00 | 20.00 |
| ATOM | 628 | N | TYR | 64 | 39.856 | 17.187 | 60.289 | 1.00 | 20.00 |
| ATOM | 630 | CA | TYR | 64 | 38.849 | 16.189 | 60.073 | 1.00 | 20.00 |
| ATOM | 631 | CB | TYR | 64 | 37.728 | 16.639 | 59.114 | 1.00 | 20.00 |
| ATOM | 632 | CG | TYR | 64 | 38.295 | 16.800 | 57.741 | 1.00 | 20.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 633 | CD1 | TYR | 64 | 38.320 | 15.737 | 56.867 | 1.00 | 20.00 |
| ATOM | 634 | CE1 | TYR | 64 | 38.835 | 15.874 | 55.599 | 1.00 | 20.00 |
| ATOM | 635 | CD2 | TYR | 64 | 38.791 | 18.013 | 57.320 | 1.00 | 20.00 |
| ATOM | 636 | CE2 | TYR | 64 | 39.310 | 18.157 | 56.054 | 1.00 | 20.00 |
| ATOM | 637 | CZ | TYR | 64 | 39.335 | 17.086 | 55.193 | 1.00 | 20.00 |
| ATOM | 638 | OH | TYR | 64 | 39.880 | 17.228 | 53.899 | 1.00 | 20.00 |
| ATOM | 640 | C | TYR | 64 | 39.501 | 14.990 | 59.462 | 1.00 | 20.00 |
| ATOM | 641 | O | TYR | 64 | 40.654 | 15.050 | 59.040 | 1.00 | 20.00 |
| ATOM | 642 | N | VAL | 65 | 38.779 | 13.849 | 59.438 | 1.00 | 20.00 |
| ATOM | 644 | CA | VAL | 65 | 39.311 | 12.653 | 58.845 | 1.00 | 20.00 |
| ATOM | 645 | CB | VAL | 65 | 39.362 | 11.494 | 59.793 | 1.00 | 20.00 |
| ATOM | 646 | CG1 | VAL | 65 | 39.871 | 10.259 | 59.032 | 1.00 | 20.00 |
| ATOM | 647 | CG2 | VAL | 65 | 40.235 | 11.888 | 60.997 | 1.00 | 20.00 |
| ATOM | 648 | C | VAL | 65 | 38.415 | 12.249 | 57.708 | 1.00 | 20.00 |
| ATOM | 649 | O | VAL | 65 | 37.194 | 12.259 | 57.835 | 1.00 | 20.00 |
| ATOM | 650 | N | LEU | 66 | 39.004 | 11.884 | 56.549 | 1.00 | 20.00 |
| ATOM | 652 | CA | LEU | 66 | 38.207 | 11.501 | 55.412 | 1.00 | 20.00 |
| ATOM | 653 | CB | LEU | 66 | 38.272 | 12.530 | 54.268 | 1.00 | 20.00 |
| ATOM | 654 | CG | LEU | 66 | 37.431 | 12.161 | 53.034 | 1.00 | 20.00 |
| ATOM | 655 | CD1 | LEU | 66 | 35.934 | 12.089 | 53.374 | 1.00 | 20.00 |
| ATOM | 656 | CD2 | LEU | 66 | 37.726 | 13.110 | 51.858 | 1.00 | 20.00 |
| ATOM | 657 | C | LEU | 66 | 38.691 | 10.186 | 54.867 | 1.00 | 20.00 |
| ATOM | 658 | O | LEU | 66 | 39.892 | 9.925 | 54.848 | 1.00 | 20.00 |
| ATOM | 659 | N | ILE | 67 | 37.758 | 9.312 | 54.410 | 1.00 | 20.00 |
| ATOM | 661 | CA | ILE | 67 | 38.160 | 8.028 | 53.887 | 1.00 | 20.00 |
| ATOM | 662 | CB | ILE | 67 | 38.248 | 6.965 | 54.942 | 1.00 | 20.00 |
| ATOM | 663 | CG2 | ILE | 67 | 39.328 | 7.382 | 55.955 | 1.00 | 20.00 |
| ATOM | 664 | CG1 | ILE | 67 | 36.866 | 6.722 | 55.570 | 1.00 | 20.00 |
| ATOM | 665 | CD1 | ILE | 67 | 36.803 | 5.463 | 56.434 | 1.00 | 20.00 |
| ATOM | 666 | C | ILE | 67 | 37.214 | 7.495 | 52.835 | 1.00 | 20.00 |
| ATOM | 667 | O | ILE | 67 | 36.047 | 7.879 | 52.768 | 1.00 | 20.00 |
| ATOM | 668 | N | ALA | 68 | 37.738 | 6.584 | 51.975 | 1.00 | 40.00 |
| ATOM | 670 | CA | ALA | 68 | 37.034 | 5.902 | 50.920 | 1.00 | 40.00 |
| ATOM | 671 | CB | ALA | 68 | 36.603 | 6.825 | 49.767 | 1.00 | 40.00 |
| ATOM | 672 | C | ALA | 68 | 38.026 | 4.927 | 50.364 | 1.00 | 40.00 |
| ATOM | 673 | O | ALA | 68 | 38.926 | 5.308 | 49.616 | 1.00 | 40.00 |
| ATOM | 674 | N | LEU | 69 | 37.895 | 3.634 | 50.721 | 1.00 | 40.00 |
| ATOM | 676 | CA | LEU | 69 | 38.868 | 2.675 | 50.282 | 1.00 | 40.00 |
| ATOM | 677 | CB | LEU | 69 | 39.908 | 2.322 | 51.360 | 1.00 | 40.00 |
| ATOM | 678 | CG | LEU | 69 | 40.796 | 3.485 | 51.840 | 1.00 | 40.00 |
| ATOM | 679 | CD1 | LEU | 69 | 39.979 | 4.582 | 52.541 | 1.00 | 40.00 |
| ATOM | 680 | CD2 | LEU | 69 | 41.929 | 2.963 | 52.738 | 1.00 | 40.00 |
| ATOM | 681 | C | LEU | 69 | 38.173 | 1.386 | 49.995 | 1.00 | 40.00 |
| ATOM | 682 | O | LEU | 69 | 36.949 | 1.285 | 50.065 | 1.00 | 40.00 |
| ATOM | 683 | N | ASN | 70 | 38.970 | 0.364 | 49.626 | 1.00 | 20.00 |
| ATOM | 685 | CA | ASN | 70 | 38.448 | -0.949 | 49.395 | 1.00 | 20.00 |
| ATOM | 686 | CB | ASN | 70 | 38.493 | -1.389 | 47.922 | 1.00 | 20.00 |
| ATOM | 687 | CG | ASN | 70 | 37.404 | -0.633 | 47.175 | 1.00 | 20.00 |
| ATOM | 688 | OD1 | ASN | 70 | 36.218 | -0.806 | 47.450 | 1.00 | 20.00 |
| ATOM | 689 | ND2 | ASN | 70 | 37.813 | 0.230 | 46.207 | 1.00 | 20.00 |
| ATOM | 692 | C | ASN | 70 | 39.314 | -1.885 | 50.172 | 1.00 | 20.00 |
| ATOM | 693 | O | ASN | 70 | 40.387 | -1.505 | 50.640 | 1.00 | 20.00 |
| ATOM | 694 | N | THR | 71 | 38.830 | -3.132 | 50.348 | 1.00 | 20.00 |
| ATOM | 696 | CA | THR | 71 | 39.493 | -4.195 | 51.056 | 1.00 | 20.00 |
| ATOM | 697 | CB | THR | 71 | 40.639 | -4.813 | 50.298 | 1.00 | 20.00 |
| ATOM | 698 | OG1 | THR | 71 | 41.089 | -5.980 | 50.970 | 1.00 | 20.00 |
| ATOM | 700 | CG2 | THR | 71 | 41.786 | -3.803 | 50.147 | 1.00 | 20.00 |
| ATOM | 701 | C | THR | 71 | 39.925 | -3.813 | 52.440 | 1.00 | 20.00 |
| ATOM | 702 | O | THR | 71 | 40.538 | -4.614 | 53.145 | 1.00 | 20.00 |
| ATOM | 703 | N | VAL | 72 | 39.580 | -2.590 | 52.888 | 1.00 | 20.00 |
| ATOM | 705 | CA | VAL | 72 | 39.932 | -2.171 | 54.215 | 1.00 | 20.00 |
| ATOM | 706 | CB | VAL | 72 | 40.149 | -0.691 | 54.328 | 1.00 | 20.00 |
| ATOM | 707 | CG1 | VAL | 72 | 40.470 | -0.349 | 55.792 | 1.00 | 20.00 |
| ATOM | 708 | CG2 | VAL | 72 | 41.247 | -0.280 | 53.333 | 1.00 | 20.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 709 | C | VAL | 72 | 38.758 | -2.514 | 55.074 | 1.00 | 20.00 |
| ATOM | 710 | O | VAL | 72 | 37.671 | -1.965 | 54.911 | 1.00 | 20.00 |
| ATOM | 711 | N | GLU | 73 | 38.955 | -3.480 | 55.988 | 1.00 | 20.00 |
| ATOM | 713 | CA | GLU | 73 | 37.923 | -3.967 | 56.856 | 1.00 | 20.00 |
| ATOM | 714 | CB | GLU | 73 | 38.349 | -5.279 | 57.534 | 1.00 | 20.00 |
| ATOM | 715 | CG | GLU | 73 | 38.561 | -6.403 | 56.516 | 1.00 | 20.00 |
| ATOM | 716 | CD | GLU | 73 | 39.076 | -7.630 | 57.251 | 1.00 | 20.00 |
| ATOM | 717 | OE1 | GLU | 73 | 39.263 | -7.542 | 58.493 | 1.00 | 20.00 |
| ATOM | 718 | OE2 | GLU | 73 | 39.289 | -8.674 | 56.578 | 1.00 | 20.00 |
| ATOM | 719 | C | GLU | 73 | 37.499 | -3.001 | 57.921 | 1.00 | 20.00 |
| ATOM | 720 | O | GLU | 73 | 36.306 | -2.829 | 58.162 | 1.00 | 20.00 |
| ATOM | 721 | N | ARG | 74 | 38.454 | -2.328 | 58.590 | 1.00 | 20.00 |
| ATOM | 723 | CA | ARG | 74 | 38.077 | -1.471 | 59.680 | 1.00 | 20.00 |
| ATOM | 724 | CB | ARG | 74 | 38.258 | -2.160 | 61.043 | 1.00 | 20.00 |
| ATOM | 725 | CG | ARG | 74 | 37.398 | -3.418 | 61.198 | 1.00 | 20.00 |
| ATOM | 726 | CD | ARG | 74 | 37.779 | -4.286 | 62.399 | 1.00 | 20.00 |
| ATOM | 727 | NE | ARG | 74 | 39.121 | -4.874 | 62.119 | 1.00 | 20.00 |
| ATOM | 729 | CZ | ARG | 74 | 40.196 | -4.529 | 62.887 | 1.00 | 20.00 |
| ATOM | 730 | NH1 | ARG | 74 | 40.047 | -3.644 | 63.915 | 1.00 | 20.00 |
| ATOM | 733 | NH2 | ARG | 74 | 41.422 | -5.075 | 62.631 | 1.00 | 20.00 |
| ATOM | 736 | C | ARG | 74 | 38.988 | -0.290 | 59.663 | 1.00 | 20.00 |
| ATOM | 737 | O | ARG | 74 | 39.927 | -0.235 | 58.875 | 1.00 | 20.00 |
| ATOM | 738 | N | ILE | 75 | 38.743 | 0.708 | 60.536 | 1.00 | 20.00 |
| ATOM | 740 | CA | ILE | 75 | 39.646 | 1.827 | 60.611 | 1.00 | 20.00 |
| ATOM | 741 | CB | ILE | 75 | 38.942 | 3.150 | 60.486 | 1.00 | 20.00 |
| ATOM | 742 | CG2 | ILE | 75 | 39.993 | 4.273 | 60.555 | 1.00 | 20.00 |
| ATOM | 743 | CG1 | ILE | 75 | 38.138 | 3.193 | 59.175 | 1.00 | 20.00 |
| ATOM | 744 | CD1 | ILE | 75 | 39.003 | 3.053 | 57.923 | 1.00 | 20.00 |
| ATOM | 745 | C | ILE | 75 | 40.260 | 1.740 | 61.980 | 1.00 | 20.00 |
| ATOM | 746 | O | ILE | 75 | 40.265 | 2.684 | 62.765 | 1.00 | 20.00 |
| ATOM | 747 | N | PRO | 76 | 40.856 | 0.609 | 62.211 | 1.00 | 20.00 |
| ATOM | 748 | CD | PRO | 76 | 41.577 | -0.084 | 61.161 | 1.00 | 20.00 |
| ATOM | 749 | CA | PRO | 76 | 41.328 | 0.159 | 63.486 | 1.00 | 20.00 |
| ATOM | 750 | CB | PRO | 76 | 41.810 | -1.276 | 63.244 | 1.00 | 20.00 |
| ATOM | 751 | CG | PRO | 76 | 41.661 | -1.506 | 61.724 | 1.00 | 20.00 |
| ATOM | 752 | C | PRO | 76 | 42.464 | 0.947 | 64.063 | 1.00 | 20.00 |
| ATOM | 753 | O | PRO | 76 | 43.009 | 0.430 | 65.036 | 1.00 | 20.00 |
| ATOM | 754 | N | LEU | 77 | 42.891 | 2.094 | 63.463 | 1.00 | 20.00 |
| ATOM | 756 | CA | LEU | 77 | 43.941 | 2.919 | 64.023 | 1.00 | 20.00 |
| ATOM | 757 | CB | LEU | 77 | 43.971 | 4.354 | 63.475 | 1.00 | 20.00 |
| ATOM | 758 | CG | LEU | 77 | 44.267 | 4.436 | 61.970 | 1.00 | 20.00 |
| ATOM | 759 | CD1 | LEU | 77 | 43.148 | 3.768 | 61.153 | 1.00 | 20.00 |
| ATOM | 760 | CD2 | LEU | 77 | 44.552 | 5.887 | 61.547 | 1.00 | 20.00 |
| ATOM | 761 | C | LEU | 77 | 43.653 | 3.019 | 65.485 | 1.00 | 20.00 |
| ATOM | 762 | O | LEU | 77 | 42.773 | 3.760 | 65.919 | 1.00 | 20.00 |
| ATOM | 763 | N | GLU | 78 | 44.422 | 2.245 | 66.273 | 1.00 | 20.00 |
| ATOM | 765 | CA | GLU | 78 | 44.154 | 2.030 | 67.661 | 1.00 | 20.00 |
| ATOM | 766 | CB | GLU | 78 | 45.215 | 1.126 | 68.313 | 1.00 | 20.00 |
| ATOM | 767 | CG | GLU | 78 | 45.162 | -0.337 | 67.872 | 1.00 | 20.00 |
| ATOM | 768 | CD | GLU | 78 | 44.210 | -1.063 | 68.810 | 1.00 | 20.00 |
| ATOM | 769 | OE1 | GLU | 78 | 43.065 | -0.569 | 68.991 | 1.00 | 20.00 |
| ATOM | 770 | OE2 | GLU | 78 | 44.620 | -2.117 | 69.367 | 1.00 | 20.00 |
| ATOM | 771 | C | GLU | 78 | 44.131 | 3.271 | 68.485 | 1.00 | 20.00 |
| ATOM | 772 | O | GLU | 78 | 43.173 | 3.510 | 69.214 | 1.00 | 20.00 |
| ATOM | 773 | N | ASN | 79 | 45.182 | 4.097 | 68.380 | 1.00 | 20.00 |
| ATOM | 775 | CA | ASN | 79 | 45.370 | 5.233 | 69.236 | 1.00 | 20.00 |
| ATOM | 776 | CB | ASN | 79 | 46.830 | 5.720 | 69.251 | 1.00 | 20.00 |
| ATOM | 777 | CG | ASN | 79 | 47.647 | 4.686 | 70.016 | 1.00 | 20.00 |
| ATOM | 778 | OD1 | ASN | 79 | 48.858 | 4.827 | 70.181 | 1.00 | 20.00 |
| ATOM | 779 | ND2 | ASN | 79 | 46.968 | 3.609 | 70.494 | 1.00 | 20.00 |
| ATOM | 782 | C | ASN | 79 | 44.505 | 6.442 | 69.057 | 1.00 | 20.00 |
| ATOM | 783 | O | ASN | 79 | 44.285 | 7.157 | 70.033 | 1.00 | 20.00 |
| ATOM | 784 | N | LEU | 80 | 44.011 | 6.718 | 67.831 | 1.00 | 20.00 |
| ATOM | 786 | CA | LEU | 80 | 43.334 | 7.957 | 67.532 | 1.00 | 20.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 787 | CB | LEU | 80 | 42.657 | 7.950 | 66.151 | 1.00 | 20.00 |
| ATOM | 788 | CG | LEU | 80 | 42.050 | 9.307 | 65.757 | 1.00 | 20.00 |
| ATOM | 789 | CD1 | LEU | 80 | 43.147 | 10.376 | 65.627 | 1.00 | 20.00 |
| ATOM | 790 | CD2 | LEU | 80 | 41.188 | 9.195 | 64.492 | 1.00 | 20.00 |
| ATOM | 791 | C | LEU | 80 | 42.315 | 8.342 | 68.565 | 1.00 | 20.00 |
| ATOM | 792 | O | LEU | 80 | 41.225 | 7.776 | 68.629 | 1.00 | 20.00 |
| ATOM | 793 | N | GLN | 81 | 42.728 | 9.271 | 69.461 | 1.00 | 20.00 |
| ATOM | 795 | CA | GLN | 81 | 41.964 | 9.831 | 70.544 | 1.00 | 20.00 |
| ATOM | 796 | CB | GLN | 81 | 42.877 | 10.381 | 71.654 | 1.00 | 20.00 |
| ATOM | 797 | CG | GLN | 81 | 43.812 | 9.339 | 72.267 | 1.00 | 20.00 |
| ATOM | 798 | CD | GLN | 81 | 42.971 | 8.360 | 73.071 | 1.00 | 20.00 |
| ATOM | 799 | OE1 | GLN | 81 | 41.955 | 8.730 | 73.659 | 1.00 | 20.00 |
| ATOM | 800 | NE2 | GLN | 81 | 43.406 | 7.072 | 73.096 | 1.00 | 20.00 |
| ATOM | 803 | C | GLN | 81 | 40.993 | 10.945 | 70.241 | 1.00 | 20.00 |
| ATOM | 804 | O | GLN | 81 | 39.869 | 10.940 | 70.741 | 1.00 | 20.00 |
| ATOM | 805 | N | ILE | 82 | 41.401 | 11.959 | 69.443 | 1.00 | 20.00 |
| ATOM | 807 | CA | ILE | 82 | 40.535 | 13.097 | 69.267 | 1.00 | 20.00 |
| ATOM | 808 | CB | ILE | 82 | 40.842 | 14.181 | 70.259 | 1.00 | 20.00 |
| ATOM | 809 | CG2 | ILE | 82 | 39.994 | 15.403 | 69.898 | 1.00 | 20.00 |
| ATOM | 810 | CG1 | ILE | 82 | 40.626 | 13.682 | 71.699 | 1.00 | 20.00 |
| ATOM | 811 | CD1 | ILE | 82 | 39.183 | 13.280 | 72.002 | 1.00 | 20.00 |
| ATOM | 812 | C | ILE | 82 | 40.686 | 13.698 | 67.897 | 1.00 | 20.00 |
| ATOM | 813 | O | ILE | 82 | 41.764 | 13.658 | 67.307 | 1.00 | 20.00 |
| ATOM | 814 | N | ILE | 83 | 39.580 | 14.259 | 67.352 | 1.00 | 20.00 |
| ATOM | 816 | CA | ILE | 83 | 39.588 | 14.935 | 66.082 | 1.00 | 20.00 |
| ATOM | 817 | CB | ILE | 83 | 38.670 | 14.293 | 65.081 | 1.00 | 20.00 |
| ATOM | 818 | CG2 | ILE | 83 | 38.638 | 15.171 | 63.821 | 1.00 | 20.00 |
| ATOM | 819 | CG1 | ILE | 83 | 39.099 | 12.841 | 64.812 | 1.00 | 20.00 |
| ATOM | 820 | CD1 | ILE | 83 | 38.048 | 12.026 | 64.060 | 1.00 | 20.00 |
| ATOM | 821 | C | ILE | 83 | 39.032 | 16.298 | 66.376 | 1.00 | 20.00 |
| ATOM | 822 | O | ILE | 83 | 37.822 | 16.488 | 66.434 | 1.00 | 20.00 |
| ATOM | 823 | N | ARG | 84 | 39.907 | 17.309 | 66.484 | 1.00 | 20.00 |
| ATOM | 825 | CA | ARG | 84 | 39.536 | 18.627 | 66.922 | 1.00 | 20.00 |
| ATOM | 826 | CB | ARG | 84 | 40.749 | 19.570 | 66.962 | 1.00 | 20.00 |
| ATOM | 827 | CG | ARG | 84 | 41.796 | 19.151 | 67.993 | 1.00 | 20.00 |
| ATOM | 828 | CD | ARG | 84 | 43.065 | 20.005 | 67.955 | 1.00 | 20.00 |
| ATOM | 829 | NE | ARG | 84 | 42.674 | 21.408 | 68.266 | 1.00 | 20.00 |
| ATOM | 831 | CZ | ARG | 84 | 42.606 | 21.830 | 69.563 | 1.00 | 20.00 |
| ATOM | 832 | NH1 | ARG | 84 | 42.894 | 20.965 | 70.579 | 1.00 | 20.00 |
| ATOM | 835 | NH2 | ARG | 84 | 42.252 | 23.118 | 69.842 | 1.00 | 20.00 |
| ATOM | 838 | C | ARG | 84 | 38.485 | 19.300 | 66.091 | 1.00 | 20.00 |
| ATOM | 839 | O | ARG | 84 | 37.694 | 20.079 | 66.618 | 1.00 | 20.00 |
| ATOM | 840 | N | GLY | 85 | 38.462 | 19.077 | 64.768 | 1.00 | 20.00 |
| ATOM | 842 | CA | GLY | 85 | 37.451 | 19.713 | 63.971 | 1.00 | 20.00 |
| ATOM | 843 | C | GLY | 85 | 37.729 | 21.178 | 63.827 | 1.00 | 20.00 |
| ATOM | 844 | O | GLY | 85 | 36.814 | 21.971 | 63.607 | 1.00 | 20.00 |
| ATOM | 845 | N | ASN | 86 | 39.009 | 21.579 | 63.922 | 1.00 | 20.00 |
| ATOM | 847 | CA | ASN | 86 | 39.344 | 22.971 | 63.806 | 1.00 | 20.00 |
| ATOM | 848 | CB | ASN | 86 | 40.860 | 23.225 | 63.837 | 1.00 | 20.00 |
| ATOM | 849 | CG | ASN | 86 | 41.372 | 22.841 | 65.216 | 1.00 | 20.00 |
| ATOM | 850 | OD1 | ASN | 86 | 40.593 | 22.557 | 66.124 | 1.00 | 20.00 |
| ATOM | 851 | ND2 | ASN | 86 | 42.722 | 22.838 | 65.381 | 1.00 | 20.00 |
| ATOM | 854 | C | ASN | 86 | 38.845 | 23.418 | 62.473 | 1.00 | 20.00 |
| ATOM | 855 | O | ASN | 86 | 38.279 | 24.503 | 62.339 | 1.00 | 20.00 |
| ATOM | 856 | N | MET | 87 | 39.054 | 22.584 | 61.441 | 1.00 | 20.00 |
| ATOM | 858 | CA | MET | 87 | 38.530 | 22.905 | 60.148 | 1.00 | 20.00 |
| ATOM | 859 | CB | MET | 87 | 39.596 | 23.081 | 59.054 | 1.00 | 20.00 |
| ATOM | 860 | CG | MET | 87 | 40.482 | 21.853 | 58.857 | 1.00 | 20.00 |
| ATOM | 861 | SD | MET | 87 | 41.713 | 21.605 | 60.170 | 1.00 | 20.00 |
| ATOM | 862 | CE | MET | 87 | 42.788 | 22.960 | 59.615 | 1.00 | 20.00 |
| ATOM | 863 | C | MET | 87 | 37.681 | 21.741 | 59.775 | 1.00 | 20.00 |
| ATOM | 864 | O | MET | 87 | 38.064 | 20.591 | 59.980 | 1.00 | 20.00 |
| ATOM | 865 | N | TYR | 88 | 36.497 | 22.022 | 59.204 | 1.00 | 20.00 |
| ATOM | 867 | CA | TYR | 88 | 35.560 | 20.985 | 58.901 | 1.00 | 20.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 868 | CB | TYR | 88 | 34.142 | 21.317 | 59.393 | 1.00 | 20.00 |
| ATOM | 869 | CG | TYR | 88 | 33.731 | 22.569 | 58.691 | 1.00 | 20.00 |
| ATOM | 870 | CD1 | TYR | 88 | 34.124 | 23.798 | 59.169 | 1.00 | 20.00 |
| ATOM | 871 | CE1 | TYR | 88 | 33.792 | 24.953 | 58.499 | 1.00 | 20.00 |
| ATOM | 872 | CD2 | TYR | 88 | 32.989 | 22.515 | 57.532 | 1.00 | 20.00 |
| ATOM | 873 | CE2 | TYR | 88 | 32.653 | 23.666 | 56.858 | 1.00 | 20.00 |
| ATOM | 874 | CZ | TYR | 88 | 33.059 | 24.887 | 57.339 | 1.00 | 20.00 |
| ATOM | 875 | OH | TYR | 88 | 32.726 | 26.069 | 56.643 | 1.00 | 20.00 |
| ATOM | 877 | C | TYR | 88 | 35.452 | 20.773 | 57.431 | 1.00 | 20.00 |
| ATOM | 878 | O | TYR | 88 | 35.783 | 21.643 | 56.625 | 1.00 | 20.00 |
| ATOM | 879 | N | TYR | 89 | 34.990 | 19.565 | 57.059 | 1.00 | 20.00 |
| ATOM | 881 | CA | TYR | 89 | 34.771 | 19.226 | 55.689 | 1.00 | 20.00 |
| ATOM | 882 | CB | TYR | 89 | 34.865 | 17.713 | 55.436 | 1.00 | 20.00 |
| ATOM | 883 | CG | TYR | 89 | 34.869 | 17.477 | 53.966 | 1.00 | 20.00 |
| ATOM | 884 | CD1 | TYR | 89 | 36.035 | 17.628 | 53.253 | 1.00 | 20.00 |
| ATOM | 885 | CE1 | TYR | 89 | 36.078 | 17.349 | 51.908 | 1.00 | 20.00 |
| ATOM | 886 | CD2 | TYR | 89 | 33.745 | 17.019 | 53.320 | 1.00 | 20.00 |
| ATOM | 887 | CE2 | TYR | 89 | 33.781 | 16.737 | 51.975 | 1.00 | 20.00 |
| ATOM | 888 | CZ | TYR | 89 | 34.949 | 16.901 | 51.269 | 1.00 | 20.00 |
| ATOM | 889 | OH | TYR | 89 | 34.989 | 16.606 | 49.890 | 1.00 | 20.00 |
| ATOM | 891 | C | TYR | 89 | 33.357 | 19.658 | 55.493 | 1.00 | 20.00 |
| ATOM | 892 | O | TYR | 89 | 32.594 | 19.687 | 56.458 | 1.00 | 20.00 |
| ATOM | 893 | N | GLU | 90 | 32.995 | 20.007 | 54.240 | 1.00 | 20.00 |
| ATOM | 895 | CA | GLU | 90 | 31.712 | 20.544 | 53.872 | 1.00 | 20.00 |
| ATOM | 896 | CB | GLU | 90 | 31.383 | 20.403 | 52.373 | 1.00 | 20.00 |
| ATOM | 897 | CG | GLU | 90 | 32.243 | 21.273 | 51.449 | 1.00 | 20.00 |
| ATOM | 898 | CD | GLU | 90 | 33.488 | 20.498 | 51.031 | 1.00 | 20.00 |
| ATOM | 899 | OE1 | GLU | 90 | 33.999 | 19.684 | 51.845 | 1.00 | 20.00 |
| ATOM | 900 | OE2 | GLU | 90 | 33.942 | 20.710 | 49.875 | 1.00 | 20.00 |
| ATOM | 901 | C | GLU | 90 | 30.596 | 19.920 | 54.637 | 1.00 | 20.00 |
| ATOM | 902 | O | GLU | 90 | 30.669 | 18.760 | 55.034 | 1.00 | 20.00 |
| ATOM | 903 | N | ASN | 91 | 29.540 | 20.711 | 54.890 | 1.00 | 20.00 |
| ATOM | 905 | CA | ASN | 91 | 28.425 | 20.266 | 55.671 | 1.00 | 20.00 |
| ATOM | 906 | CB | ASN | 91 | 27.743 | 19.004 | 55.118 | 1.00 | 20.00 |
| ATOM | 907 | CG | ASN | 91 | 26.376 | 18.884 | 55.782 | 1.00 | 20.00 |
| ATOM | 908 | OD1 | ASN | 91 | 26.067 | 19.584 | 56.745 | 1.00 | 20.00 |
| ATOM | 909 | ND2 | ASN | 91 | 25.526 | 17.968 | 55.247 | 1.00 | 20.00 |
| ATOM | 912 | C | ASN | 91 | 28.955 | 19.976 | 57.037 | 1.00 | 20.00 |
| ATOM | 913 | O | ASN | 91 | 28.340 | 19.265 | 57.830 | 1.00 | 20.00 |
| ATOM | 914 | N | SER | 92 | 30.120 | 20.575 | 57.343 | 1.00 | 20.00 |
| ATOM | 916 | CA | SER | 92 | 30.775 | 20.462 | 58.611 | 1.00 | 20.00 |
| ATOM | 917 | CB | SER | 92 | 30.121 | 21.328 | 59.705 | 1.00 | 20.00 |
| ATOM | 918 | OG | SER | 92 | 28.804 | 20.867 | 59.972 | 1.00 | 20.00 |
| ATOM | 920 | C | SER | 92 | 30.861 | 19.058 | 59.117 | 1.00 | 20.00 |
| ATOM | 921 | O | SER | 92 | 30.223 | 18.715 | 60.111 | 1.00 | 20.00 |
| ATOM | 922 | N | TYR | 93 | 31.668 | 18.203 | 58.453 | 1.00 | 20.00 |
| ATOM | 924 | CA | TYR | 93 | 31.828 | 16.876 | 58.966 | 1.00 | 20.00 |
| ATOM | 925 | CB | TYR | 93 | 31.560 | 15.753 | 57.946 | 1.00 | 20.00 |
| ATOM | 926 | CG | TYR | 93 | 30.103 | 15.728 | 57.618 | 1.00 | 20.00 |
| ATOM | 927 | CD1 | TYR | 93 | 29.612 | 16.358 | 56.497 | 1.00 | 20.00 |
| ATOM | 928 | CE1 | TYR | 93 | 28.270 | 16.311 | 56.196 | 1.00 | 20.00 |
| ATOM | 929 | CD2 | TYR | 93 | 29.220 | 15.080 | 58.452 | 1.00 | 20.00 |
| ATOM | 930 | CE2 | TYR | 93 | 27.876 | 15.039 | 58.163 | 1.00 | 20.00 |
| ATOM | 931 | CZ | TYR | 93 | 27.400 | 15.650 | 57.028 | 1.00 | 20.00 |
| ATOM | 932 | OH | TYR | 93 | 26.023 | 15.603 | 56.722 | 1.00 | 20.00 |
| ATOM | 934 | C | TYR | 93 | 33.237 | 16.716 | 59.448 | 1.00 | 20.00 |
| ATOM | 935 | O | TYR | 93 | 34.195 | 17.026 | 58.744 | 1.00 | 20.00 |
| ATOM | 936 | N | ALA | 94 | 33.384 | 16.307 | 60.722 | 1.00 | 20.00 |
| ATOM | 938 | CA | ALA | 94 | 34.651 | 16.026 | 61.332 | 1.00 | 20.00 |
| ATOM | 939 | CB | ALA | 94 | 34.568 | 15.964 | 62.866 | 1.00 | 20.00 |
| ATOM | 940 | C | ALA | 94 | 35.172 | 14.706 | 60.866 | 1.00 | 20.00 |
| ATOM | 941 | O | ALA | 94 | 36.378 | 14.536 | 60.696 | 1.00 | 20.00 |
| ATOM | 942 | N | LEU | 95 | 34.266 | 13.724 | 60.696 | 1.00 | 20.00 |
| ATOM | 944 | CA | LEU | 95 | 34.661 | 12.411 | 60.279 | 1.00 | 20.00 |

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| ATOM | 945 | CB | LEU | 95 | 34.488 | 11.374 | 61.403 | 1.00 | 20.00 |
| ATOM | 946 | CG | LEU | 95 | 34.889 | 9.936 | 61.030 | 1.00 | 20.00 |
| ATOM | 947 | CD1 | LEU | 95 | 36.389 | 9.831 | 60.704 | 1.00 | 20.00 |
| ATOM | 948 | CD2 | LEU | 95 | 34.445 | 8.947 | 62.122 | 1.00 | 20.00 |
| ATOM | 949 | C | LEU | 95 | 33.775 | 12.005 | 59.148 | 1.00 | 20.00 |
| ATOM | 950 | O | LEU | 95 | 32.580 | 11.774 | 59.326 | 1.00 | 20.00 |
| ATOM | 951 | N | ALA | 96 | 34.344 | 11.901 | 57.934 | 1.00 | 20.00 |
| ATOM | 953 | CA | ALA | 96 | 33.529 | 11.501 | 56.828 | 1.00 | 20.00 |
| ATOM | 954 | CB | ALA | 96 | 33.592 | 12.471 | 55.636 | 1.00 | 20.00 |
| ATOM | 955 | C | ALA | 96 | 34.041 | 10.183 | 56.352 | 1.00 | 20.00 |
| ATOM | 956 | O | ALA | 96 | 35.222 | 10.053 | 56.040 | 1.00 | 20.00 |
| ATOM | 957 | N | VAL | 97 | 33.165 | 9.160 | 56.327 | 1.00 | 20.00 |
| ATOM | 959 | CA | VAL | 97 | 33.548 | 7.887 | 55.793 | 1.00 | 20.00 |
| ATOM | 960 | CB | VAL | 97 | 33.554 | 6.778 | 56.812 | 1.00 | 20.00 |
| ATOM | 961 | CG1 | VAL | 97 | 34.698 | 7.057 | 57.803 | 1.00 | 20.00 |
| ATOM | 962 | CG2 | VAL | 97 | 32.183 | 6.709 | 57.507 | 1.00 | 20.00 |
| ATOM | 963 | C | VAL | 97 | 32.560 | 7.591 | 54.706 | 1.00 | 20.00 |
| ATOM | 964 | O | VAL | 97 | 31.395 | 7.287 | 54.955 | 1.00 | 20.00 |
| ATOM | 965 | N | LEU | 98 | 33.010 | 7.671 | 53.443 | 1.00 | 20.00 |
| ATOM | 967 | CA | LEU | 98 | 32.089 | 7.495 | 52.359 | 1.00 | 20.00 |
| ATOM | 968 | CB | LEU | 98 | 32.012 | 8.718 | 51.428 | 1.00 | 20.00 |
| ATOM | 969 | CG | LEU | 98 | 31.150 | 8.489 | 50.171 | 1.00 | 20.00 |
| ATOM | 970 | CD1 | LEU | 98 | 29.683 | 8.208 | 50.525 | 1.00 | 20.00 |
| ATOM | 971 | CD2 | LEU | 98 | 31.312 | 9.645 | 49.170 | 1.00 | 20.00 |
| ATOM | 972 | C | LEU | 98 | 32.469 | 6.338 | 51.501 | 1.00 | 20.00 |
| ATOM | 973 | O | LEU | 98 | 33.649 | 6.086 | 51.273 | 1.00 | 20.00 |
| ATOM | 974 | N | SER | 99 | 31.427 | 5.622 | 51.017 | 1.00 | 20.00 |
| ATOM | 976 | CA | SER | 99 | 31.533 | 4.513 | 50.113 | 1.00 | 20.00 |
| ATOM | 977 | CB | SER | 99 | 31.565 | 4.948 | 48.637 | 1.00 | 20.00 |
| ATOM | 978 | OG | SER | 99 | 31.664 | 3.812 | 47.792 | 1.00 | 20.00 |
| ATOM | 980 | C | SER | 99 | 32.738 | 3.676 | 50.385 | 1.00 | 20.00 |
| ATOM | 981 | O | SER | 99 | 33.741 | 3.777 | 49.679 | 1.00 | 20.00 |
| ATOM | 982 | N | ASN | 100 | 32.683 | 2.847 | 51.441 | 1.00 | 40.00 |
| ATOM | 984 | CA | ASN | 100 | 33.796 | 1.990 | 51.716 | 1.00 | 40.00 |
| ATOM | 985 | CB | ASN | 100 | 34.171 | 1.941 | 53.206 | 1.00 | 40.00 |
| ATOM | 986 | CG | ASN | 100 | 34.709 | 3.304 | 53.612 | 1.00 | 40.00 |
| ATOM | 987 | OD1 | ASN | 100 | 34.075 | 4.033 | 54.371 | 1.00 | 40.00 |
| ATOM | 988 | ND2 | ASN | 100 | 35.912 | 3.661 | 53.088 | 1.00 | 40.00 |
| ATOM | 991 | C | ASN | 100 | 33.361 | 0.605 | 51.348 | 1.00 | 40.00 |
| ATOM | 992 | O | ASN | 100 | 32.801 | -0.113 | 52.172 | 1.00 | 40.00 |
| ATOM | 993 | N | TYR | 101 | 33.630 | 0.186 | 50.097 | 1.00 | 40.00 |
| ATOM | 995 | CA | TYR | 101 | 33.219 | -1.112 | 49.639 | 1.00 | 40.00 |
| ATOM | 996 | CB | TYR | 101 | 32.957 | -1.200 | 48.122 | 1.00 | 40.00 |
| ATOM | 997 | CG | TYR | 101 | 31.781 | -0.366 | 47.741 | 1.00 | 40.00 |
| ATOM | 998 | CD1 | TYR | 101 | 30.502 | -0.820 | 47.972 | 1.00 | 40.00 |
| ATOM | 999 | CE1 | TYR | 101 | 29.415 | -0.125 | 47.495 | 1.00 | 40.00 |
| ATOM | 1000 | CD2 | TYR | 101 | 31.958 | 0.775 | 46.992 | 1.00 | 40.00 |
| ATOM | 1001 | CE2 | TYR | 101 | 30.875 | 1.470 | 46.507 | 1.00 | 40.00 |
| ATOM | 1002 | CZ | TYR | 101 | 29.601 | 1.021 | 46.761 | 1.00 | 40.00 |
| ATOM | 1003 | OH | TYR | 101 | 28.489 | 1.723 | 46.251 | 1.00 | 40.00 |
| ATOM | 1005 | C | TYR | 101 | 34.312 | -2.096 | 49.893 | 1.00 | 40.00 |
| ATOM | 1006 | O | TYR | 101 | 35.170 | -1.894 | 50.752 | 1.00 | 40.00 |
| ATOM | 1007 | N | ASP | 102 | 34.256 | -3.225 | 49.153 | 1.00 | 60.00 |
| ATOM | 1009 | CA | ASP | 102 | 35.256 | -4.250 | 49.221 | 1.00 | 60.00 |
| ATOM | 1010 | CB | ASP | 102 | 34.979 | -5.334 | 50.276 | 1.00 | 60.00 |
| ATOM | 1011 | CG | ASP | 102 | 36.283 | -6.075 | 50.550 | 1.00 | 60.00 |
| ATOM | 1012 | OD1 | ASP | 102 | 37.327 | -5.662 | 49.979 | 1.00 | 60.00 |
| ATOM | 1013 | OD2 | ASP | 102 | 36.252 | -7.065 | 51.329 | 1.00 | 60.00 |
| ATOM | 1014 | C | ASP | 102 | 35.215 | -4.938 | 47.893 | 1.00 | 60.00 |
| ATOM | 1015 | O | ASP | 102 | 34.499 | -4.515 | 46.986 | 1.00 | 60.00 |
| ATOM | 1016 | N | ALA | 103 | 36.007 | -6.017 | 47.742 | 1.00 | 60.00 |
| ATOM | 1018 | CA | ALA | 103 | 36.008 | -6.756 | 46.516 | 1.00 | 60.00 |
| ATOM | 1019 | CB | ALA | 103 | 37.015 | -7.919 | 46.523 | 1.00 | 60.00 |
| ATOM | 1020 | C | ALA | 103 | 34.647 | -7.347 | 46.359 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1021 | O | ALA | 103 | 34.025 | -7.233 | 45.304 | 1.00 | 60.00 |
| ATOM | 1022 | N | ASN | 104 | 34.138 | -7.984 | 47.430 | 1.00 | 60.00 |
| ATOM | 1024 | CA | ASN | 104 | 32.835 | -8.569 | 47.350 | 1.00 | 60.00 |
| ATOM | 1025 | CB | ASN | 104 | 32.720 | -9.946 | 48.030 | 1.00 | 60.00 |
| ATOM | 1026 | CG | ASN | 104 | 32.998 | -9.784 | 49.516 | 1.00 | 60.00 |
| ATOM | 1027 | OD1 | ASN | 104 | 32.112 | -9.433 | 50.294 | 1.00 | 60.00 |
| ATOM | 1028 | ND2 | ASN | 104 | 34.266 | -10.058 | 49.926 | 1.00 | 60.00 |
| ATOM | 1031 | C | ASN | 104 | 31.884 | -7.637 | 48.020 | 1.00 | 60.00 |
| ATOM | 1032 | O | ASN | 104 | 32.185 | -6.462 | 48.219 | 1.00 | 60.00 |
| ATOM | 1033 | N | LYS | 105 | 30.692 | -8.148 | 48.379 | 1.00 | 60.00 |
| ATOM | 1035 | CA | LYS | 105 | 29.702 | -7.312 | 48.989 | 1.00 | 60.00 |
| ATOM | 1036 | CB | LYS | 105 | 28.296 | -7.937 | 48.947 | 1.00 | 60.00 |
| ATOM | 1037 | CG | LYS | 105 | 27.168 | -6.984 | 49.345 | 1.00 | 60.00 |
| ATOM | 1038 | CD | LYS | 105 | 25.778 | -7.506 | 48.968 | 1.00 | 60.00 |
| ATOM | 1039 | CE | LYS | 105 | 25.542 | -7.581 | 47.458 | 1.00 | 60.00 |
| ATOM | 1040 | NZ | LYS | 105 | 24.184 | -8.102 | 47.179 | 1.00 | 60.00 |
| ATOM | 1044 | C | LYS | 105 | 30.074 | -7.109 | 50.420 | 1.00 | 60.00 |
| ATOM | 1045 | O | LYS | 105 | 29.596 | -7.823 | 51.301 | 1.00 | 60.00 |
| ATOM | 1046 | N | THR | 106 | 30.953 | -6.121 | 50.683 | 1.00 | 60.00 |
| ATOM | 1048 | CA | THR | 106 | 31.369 | -5.845 | 52.027 | 1.00 | 60.00 |
| ATOM | 1049 | CB | THR | 106 | 31.793 | -7.084 | 52.771 | 1.00 | 60.00 |
| ATOM | 1050 | OG1 | THR | 106 | 31.980 | -6.802 | 54.151 | 1.00 | 60.00 |
| ATOM | 1052 | CG2 | THR | 106 | 33.086 | -7.635 | 52.145 | 1.00 | 60.00 |
| ATOM | 1053 | C | THR | 106 | 32.528 | -4.897 | 51.936 | 1.00 | 60.00 |
| ATOM | 1054 | O | THR | 106 | 32.620 | -4.105 | 51.000 | 1.00 | 60.00 |
| ATOM | 1055 | N | GLY | 107 | 33.435 | -4.946 | 52.930 | 1.00 | 40.00 |
| ATOM | 1057 | CA | GLY | 107 | 34.619 | -4.142 | 52.938 | 1.00 | 40.00 |
| ATOM | 1058 | C | GLY | 107 | 34.820 | -3.603 | 54.311 | 1.00 | 40.00 |
| ATOM | 1059 | O | GLY | 107 | 35.592 | -4.153 | 55.094 | 1.00 | 40.00 |
| ATOM | 1060 | N | LEU | 108 | 34.103 | -2.527 | 54.668 | 1.00 | 20.00 |
| ATOM | 1062 | CA | LEU | 108 | 34.303 | -1.977 | 55.974 | 1.00 | 20.00 |
| ATOM | 1063 | CB | LEU | 108 | 34.097 | -0.453 | 56.025 | 1.00 | 20.00 |
| ATOM | 1064 | CG | LEU | 108 | 34.309 | 0.161 | 57.420 | 1.00 | 20.00 |
| ATOM | 1065 | CD1 | LEU | 108 | 35.765 | -0.006 | 57.885 | 1.00 | 20.00 |
| ATOM | 1066 | CD2 | LEU | 108 | 33.842 | 1.625 | 57.463 | 1.00 | 20.00 |
| ATOM | 1067 | C | LEU | 108 | 33.283 | -2.598 | 56.868 | 1.00 | 20.00 |
| ATOM | 1068 | O | LEU | 108 | 32.105 | -2.259 | 56.795 | 1.00 | 20.00 |
| ATOM | 1069 | N | LYS | 109 | 33.711 | -3.570 | 57.691 | 1.00 | 20.00 |
| ATOM | 1071 | CA | LYS | 109 | 32.849 | -4.236 | 58.625 | 1.00 | 20.00 |
| ATOM | 1072 | CB | LYS | 109 | 33.493 | -5.499 | 59.220 | 1.00 | 20.00 |
| ATOM | 1073 | CG | LYS | 109 | 33.728 | -6.599 | 58.181 | 1.00 | 20.00 |
| ATOM | 1074 | CD | LYS | 109 | 34.771 | -6.233 | 57.124 | 1.00 | 20.00 |
| ATOM | 1075 | CE | LYS | 109 | 35.007 | -7.330 | 56.084 | 1.00 | 20.00 |
| ATOM | 1076 | NZ | LYS | 109 | 35.648 | -8.503 | 56.719 | 1.00 | 20.00 |
| ATOM | 1080 | C | LYS | 109 | 32.486 | -3.335 | 59.761 | 1.00 | 20.00 |
| ATOM | 1081 | O | LYS | 109 | 31.356 | -3.352 | 60.243 | 1.00 | 20.00 |
| ATOM | 1082 | N | GLU | 110 | 33.452 | -2.532 | 60.241 | 1.00 | 20.00 |
| ATOM | 1084 | CA | GLU | 110 | 33.191 | -1.699 | 61.375 | 1.00 | 20.00 |
| ATOM | 1085 | CB | GLU | 110 | 33.243 | -2.506 | 62.686 | 1.00 | 20.00 |
| ATOM | 1086 | CG | GLU | 110 | 34.443 | -3.458 | 62.753 | 1.00 | 20.00 |
| ATOM | 1087 | CD | GLU | 110 | 34.394 | -4.215 | 64.072 | 1.00 | 20.00 |
| ATOM | 1088 | OE1 | GLU | 110 | 33.311 | -4.770 | 64.393 | 1.00 | 20.00 |
| ATOM | 1089 | OE2 | GLU | 110 | 35.438 | -4.249 | 64.776 | 1.00 | 20.00 |
| ATOM | 1090 | C | GLU | 110 | 34.192 | -0.592 | 61.413 | 1.00 | 20.00 |
| ATOM | 1091 | O | GLU | 110 | 35.084 | -0.516 | 60.570 | 1.00 | 20.00 |
| ATOM | 1092 | N | LEU | 111 | 33.987 | 0.344 | 62.363 | 1.00 | 20.00 |
| ATOM | 1094 | CA | LEU | 111 | 34.824 | 1.475 | 62.663 | 1.00 | 20.00 |
| ATOM | 1095 | CB | LEU | 111 | 34.012 | 2.581 | 63.358 | 1.00 | 20.00 |
| ATOM | 1096 | CG | LEU | 111 | 34.824 | 3.839 | 63.700 | 1.00 | 20.00 |
| ATOM | 1097 | CD1 | LEU | 111 | 35.301 | 4.544 | 62.419 | 1.00 | 20.00 |
| ATOM | 1098 | CD2 | LEU | 111 | 34.041 | 4.771 | 64.638 | 1.00 | 20.00 |
| ATOM | 1099 | C | LEU | 111 | 36.051 | 1.204 | 63.522 | 1.00 | 20.00 |
| ATOM | 1100 | O | LEU | 111 | 37.050 | 1.894 | 63.330 | 1.00 | 20.00 |
| ATOM | 1101 | N | PRO | 112 | 36.057 | 0.168 | 64.355 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1102 | CD | PRO | 112 | 36.108 | -1.117 | 63.673 | 1.00 | 20.00 |
| ATOM | 1103 | CA | PRO | 112 | 36.946 | 0.092 | 65.507 | 1.00 | 20.00 |
| ATOM | 1104 | CB | PRO | 112 | 37.607 | -1.286 | 65.523 | 1.00 | 20.00 |
| ATOM | 1105 | CG | PRO | 112 | 37.399 | -1.812 | 64.107 | 1.00 | 20.00 |
| ATOM | 1106 | C | PRO | 112 | 37.924 | 1.181 | 65.815 | 1.00 | 20.00 |
| ATOM | 1107 | O | PRO | 112 | 39.116 | 0.935 | 65.971 | 1.00 | 20.00 |
| ATOM | 1108 | N | MET | 113 | 37.371 | 2.381 | 66.007 | 1.00 | 20.00 |
| ATOM | 1110 | CA | MET | 113 | 37.969 | 3.619 | 66.401 | 1.00 | 20.00 |
| ATOM | 1111 | CB | MET | 113 | 37.208 | 4.872 | 65.938 | 1.00 | 20.00 |
| ATOM | 1112 | CG | MET | 113 | 37.357 | 5.147 | 64.443 | 1.00 | 20.00 |
| ATOM | 1113 | SD | MET | 113 | 39.035 | 5.590 | 63.905 | 1.00 | 20.00 |
| ATOM | 1114 | CE | MET | 113 | 38.968 | 7.272 | 64.579 | 1.00 | 20.00 |
| ATOM | 1115 | C | MET | 113 | 38.023 | 3.646 | 67.891 | 1.00 | 20.00 |
| ATOM | 1116 | O | MET | 113 | 38.035 | 4.725 | 68.468 | 1.00 | 20.00 |
| ATOM | 1117 | N | ARG | 114 | 37.983 | 2.481 | 68.565 | 1.00 | 20.00 |
| ATOM | 1119 | CA | ARG | 114 | 37.744 | 2.375 | 69.983 | 1.00 | 20.00 |
| ATOM | 1120 | CB | ARG | 114 | 38.199 | 1.019 | 70.550 | 1.00 | 20.00 |
| ATOM | 1121 | CG | ARG | 114 | 39.689 | 0.735 | 70.352 | 1.00 | 20.00 |
| ATOM | 1122 | CD | ARG | 114 | 39.990 | -0.125 | 69.122 | 1.00 | 20.00 |
| ATOM | 1123 | NE | ARG | 114 | 39.362 | -1.457 | 69.345 | 1.00 | 20.00 |
| ATOM | 1125 | CZ | ARG | 114 | 39.850 | -2.557 | 68.703 | 1.00 | 20.00 |
| ATOM | 1126 | NH1 | ARG | 114 | 39.275 | -3.778 | 68.906 | 1.00 | 20.00 |
| ATOM | 1129 | NH2 | ARG | 114 | 40.917 | -2.437 | 67.859 | 1.00 | 20.00 |
| ATOM | 1132 | C | ARG | 114 | 38.335 | 3.440 | 70.870 | 1.00 | 20.00 |
| ATOM | 1133 | O | ARG | 114 | 37.721 | 3.778 | 71.879 | 1.00 | 20.00 |
| ATOM | 1134 | N | ASN | 115 | 39.533 | 3.969 | 70.584 | 1.00 | 20.00 |
| ATOM | 1136 | CA | ASN | 115 | 40.116 | 5.009 | 71.396 | 1.00 | 20.00 |
| ATOM | 1137 | CB | ASN | 115 | 41.633 | 5.149 | 71.193 | 1.00 | 20.00 |
| ATOM | 1138 | CG | ASN | 115 | 42.267 | 3.951 | 71.883 | 1.00 | 20.00 |
| ATOM | 1139 | OD1 | ASN | 115 | 41.577 | 3.133 | 72.489 | 1.00 | 20.00 |
| ATOM | 1140 | ND2 | ASN | 115 | 43.619 | 3.851 | 71.812 | 1.00 | 20.00 |
| ATOM | 1143 | C | ASN | 115 | 39.483 | 6.371 | 71.233 | 1.00 | 20.00 |
| ATOM | 1144 | O | ASN | 115 | 39.737 | 7.272 | 72.029 | 1.00 | 20.00 |
| ATOM | 1145 | N | LEU | 116 | 38.690 | 6.577 | 70.164 | 1.00 | 20.00 |
| ATOM | 1147 | CA | LEU | 116 | 38.092 | 7.838 | 69.813 | 1.00 | 20.00 |
| ATOM | 1148 | CB | LEU | 116 | 37.302 | 7.771 | 68.493 | 1.00 | 20.00 |
| ATOM | 1149 | CG | LEU | 116 | 36.636 | 9.094 | 68.073 | 1.00 | 20.00 |
| ATOM | 1150 | CD1 | LEU | 116 | 37.689 | 10.176 | 67.784 | 1.00 | 20.00 |
| ATOM | 1151 | CD2 | LEU | 116 | 35.666 | 8.886 | 66.901 | 1.00 | 20.00 |
| ATOM | 1152 | C | LEU | 116 | 37.155 | 8.329 | 70.876 | 1.00 | 20.00 |
| ATOM | 1153 | O | LEU | 116 | 36.014 | 7.880 | 70.973 | 1.00 | 20.00 |
| ATOM | 1154 | N | GLN | 117 | 37.673 | 9.215 | 71.750 | 1.00 | 20.00 |
| ATOM | 1156 | CA | GLN | 117 | 36.955 | 9.843 | 72.820 | 1.00 | 20.00 |
| ATOM | 1157 | CB | GLN | 117 | 37.897 | 10.308 | 73.944 | 1.00 | 20.00 |
| ATOM | 1158 | CG | GLN | 117 | 38.698 | 9.182 | 74.599 | 1.00 | 20.00 |
| ATOM | 1159 | CD | GLN | 117 | 37.734 | 8.298 | 75.375 | 1.00 | 20.00 |
| ATOM | 1160 | OE1 | GLN | 117 | 36.848 | 7.672 | 74.795 | 1.00 | 20.00 |
| ATOM | 1161 | NE2 | GLN | 117 | 37.907 | 8.244 | 76.724 | 1.00 | 20.00 |
| ATOM | 1164 | C | GLN | 117 | 36.146 | 11.051 | 72.455 | 1.00 | 20.00 |
| ATOM | 1165 | O | GLN | 117 | 35.059 | 11.239 | 72.993 | 1.00 | 20.00 |
| ATOM | 1166 | N | GLU | 118 | 36.662 | 11.951 | 71.587 | 1.00 | 20.00 |
| ATOM | 1168 | CA | GLU | 118 | 35.860 | 13.113 | 71.321 | 1.00 | 20.00 |
| ATOM | 1169 | CB | GLU | 118 | 35.913 | 14.183 | 72.424 | 1.00 | 20.00 |
| ATOM | 1170 | CG | GLU | 118 | 34.858 | 15.275 | 72.226 | 1.00 | 20.00 |
| ATOM | 1171 | CD | GLU | 118 | 34.975 | 16.291 | 73.350 | 1.00 | 20.00 |
| ATOM | 1172 | OE1 | GLU | 118 | 33.956 | 16.974 | 73.630 | 1.00 | 20.00 |
| ATOM | 1173 | OE2 | GLU | 118 | 36.084 | 16.402 | 73.940 | 1.00 | 20.00 |
| ATOM | 1174 | C | GLU | 118 | 36.217 | 13.797 | 70.043 | 1.00 | 20.00 |
| ATOM | 1175 | O | GLU | 118 | 37.375 | 13.829 | 69.629 | 1.00 | 20.00 |
| ATOM | 1176 | N | ILE | 119 | 35.185 | 14.358 | 69.380 | 1.00 | 20.00 |
| ATOM | 1178 | CA | ILE | 119 | 35.360 | 15.138 | 68.194 | 1.00 | 20.00 |
| ATOM | 1179 | CB | ILE | 119 | 34.474 | 14.698 | 67.059 | 1.00 | 20.00 |
| ATOM | 1180 | CG2 | ILE | 119 | 34.603 | 15.722 | 65.922 | 1.00 | 20.00 |
| ATOM | 1181 | CG1 | ILE | 119 | 34.829 | 13.264 | 66.628 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1182 | CD1 | ILE | 119 | 33.826 | 12.644 | 65.654 | 1.00 | 20.00 |
| ATOM | 1183 | C | ILE | 119 | 34.944 | 16.515 | 68.607 | 1.00 | 20.00 |
| ATOM | 1184 | O | ILE | 119 | 33.767 | 16.862 | 68.525 | 1.00 | 20.00 |
| ATOM | 1185 | N | LEU | 120 | 35.925 | 17.373 | 68.955 | 1.00 | 20.00 |
| ATOM | 1187 | CA | LEU | 120 | 35.647 | 18.662 | 69.531 | 1.00 | 20.00 |
| ATOM | 1188 | CB | LEU | 120 | 36.861 | 19.604 | 69.661 | 1.00 | 20.00 |
| ATOM | 1189 | CG | LEU | 120 | 37.871 | 19.235 | 70.761 | 1.00 | 20.00 |
| ATOM | 1190 | CD1 | LEU | 120 | 38.609 | 17.938 | 70.424 | 1.00 | 20.00 |
| ATOM | 1191 | CD2 | LEU | 120 | 38.825 | 20.404 | 71.057 | 1.00 | 20.00 |
| ATOM | 1192 | C | LEU | 120 | 34.660 | 19.438 | 68.726 | 1.00 | 20.00 |
| ATOM | 1193 | O | LEU | 120 | 33.852 | 20.172 | 69.292 | 1.00 | 20.00 |
| ATOM | 1194 | N | HIS | 121 | 34.699 | 19.344 | 67.387 | 1.00 | 20.00 |
| ATOM | 1196 | CA | HIS | 121 | 33.731 | 20.124 | 66.677 | 1.00 | 20.00 |
| ATOM | 1197 | CB | HIS | 121 | 34.231 | 21.527 | 66.296 | 1.00 | 20.00 |
| ATOM | 1198 | CG | HIS | 121 | 33.162 | 22.376 | 65.673 | 1.00 | 20.00 |
| ATOM | 1199 | CD2 | HIS | 121 | 32.867 | 22.598 | 64.363 | 1.00 | 20.00 |
| ATOM | 1200 | ND1 | HIS | 121 | 32.234 | 23.095 | 66.393 | 1.00 | 20.00 |
| ATOM | 1202 | CE1 | HIS | 121 | 31.430 | 23.713 | 65.490 | 1.00 | 20.00 |
| ATOM | 1203 | NE2 | HIS | 121 | 31.776 | 23.441 | 64.245 | 1.00 | 20.00 |
| ATOM | 1205 | C | HIS | 121 | 33.334 | 19.442 | 65.411 | 1.00 | 20.00 |
| ATOM | 1206 | O | HIS | 121 | 34.098 | 18.668 | 64.840 | 1.00 | 20.00 |
| ATOM | 1207 | N | GLY | 122 | 32.099 | 19.720 | 64.947 | 1.00 | 20.00 |
| ATOM | 1209 | CA | GLY | 122 | 31.633 | 19.168 | 63.714 | 1.00 | 20.00 |
| ATOM | 1210 | C | GLY | 122 | 30.940 | 17.873 | 63.991 | 1.00 | 20.00 |
| ATOM | 1211 | O | GLY | 122 | 31.039 | 17.322 | 65.086 | 1.00 | 20.00 |
| ATOM | 1212 | N | ALA | 123 | 30.204 | 17.370 | 62.978 | 1.00 | 20.00 |
| ATOM | 1214 | CA | ALA | 123 | 29.471 | 16.140 | 63.080 | 1.00 | 20.00 |
| ATOM | 1215 | CB | ALA | 123 | 28.040 | 16.233 | 62.527 | 1.00 | 20.00 |
| ATOM | 1216 | C | ALA | 123 | 30.174 | 15.063 | 62.315 | 1.00 | 20.00 |
| ATOM | 1217 | O | ALA | 123 | 31.321 | 15.229 | 61.909 | 1.00 | 20.00 |
| ATOM | 1218 | N | VAL | 124 | 29.500 | 13.906 | 62.126 | 1.00 | 20.00 |
| ATOM | 1220 | CA | VAL | 124 | 30.075 | 12.810 | 61.392 | 1.00 | 20.00 |
| ATOM | 1221 | CB | VAL | 124 | 30.249 | 11.569 | 62.219 | 1.00 | 20.00 |
| ATOM | 1222 | CG1 | VAL | 124 | 28.855 | 11.048 | 62.614 | 1.00 | 20.00 |
| ATOM | 1223 | CG2 | VAL | 124 | 31.094 | 10.562 | 61.420 | 1.00 | 20.00 |
| ATOM | 1224 | C | VAL | 124 | 29.175 | 12.455 | 60.246 | 1.00 | 20.00 |
| ATOM | 1225 | O | VAL | 124 | 28.001 | 12.822 | 60.226 | 1.00 | 20.00 |
| ATOM | 1226 | N | ARG | 125 | 29.718 | 11.762 | 59.223 | 1.00 | 20.00 |
| ATOM | 1228 | CA | ARG | 125 | 28.902 | 11.392 | 58.101 | 1.00 | 20.00 |
| ATOM | 1229 | CB | ARG | 125 | 29.175 | 12.269 | 56.870 | 1.00 | 20.00 |
| ATOM | 1230 | CG | ARG | 125 | 28.335 | 11.918 | 55.646 | 1.00 | 20.00 |
| ATOM | 1231 | CD | ARG | 125 | 28.619 | 12.837 | 54.459 | 1.00 | 20.00 |
| ATOM | 1232 | NE | ARG | 125 | 27.732 | 12.408 | 53.345 | 1.00 | 20.00 |
| ATOM | 1234 | CZ | ARG | 125 | 26.442 | 12.852 | 53.316 | 1.00 | 20.00 |
| ATOM | 1235 | NH1 | ARG | 125 | 25.626 | 12.509 | 52.278 | 1.00 | 20.00 |
| ATOM | 1238 | NH2 | ARG | 125 | 25.966 | 13.637 | 54.325 | 1.00 | 20.00 |
| ATOM | 1241 | C | ARG | 125 | 29.243 | 9.985 | 57.723 | 1.00 | 20.00 |
| ATOM | 1242 | O | ARG | 125 | 30.297 | 9.728 | 57.145 | 1.00 | 20.00 |
| ATOM | 1243 | N | PHE | 126 | 28.354 | 9.023 | 58.025 | 1.00 | 20.00 |
| ATOM | 1245 | CA | PHE | 126 | 28.636 | 7.664 | 57.661 | 1.00 | 20.00 |
| ATOM | 1246 | CB | PHE | 126 | 28.341 | 6.650 | 58.781 | 1.00 | 20.00 |
| ATOM | 1247 | CG | PHE | 126 | 29.317 | 6.817 | 59.893 | 1.00 | 20.00 |
| ATOM | 1248 | CD1 | PHE | 126 | 30.518 | 6.145 | 59.875 | 1.00 | 20.00 |
| ATOM | 1249 | CD2 | PHE | 126 | 28.994 | 7.566 | 61.000 | 1.00 | 20.00 |
| ATOM | 1250 | CE1 | PHE | 126 | 31.389 | 6.236 | 60.934 | 1.00 | 20.00 |
| ATOM | 1251 | CE2 | PHE | 126 | 29.861 | 7.662 | 62.062 | 1.00 | 20.00 |
| ATOM | 1252 | CZ | PHE | 126 | 31.060 | 6.993 | 62.033 | 1.00 | 20.00 |
| ATOM | 1253 | C | PHE | 126 | 27.707 | 7.295 | 56.548 | 1.00 | 20.00 |
| ATOM | 1254 | O | PHE | 126 | 26.558 | 6.923 | 56.781 | 1.00 | 20.00 |
| ATOM | 1255 | N | SER | 127 | 28.193 | 7.340 | 55.295 | 1.00 | 20.00 |
| ATOM | 1257 | CA | SER | 127 | 27.298 | 7.056 | 54.219 | 1.00 | 20.00 |
| ATOM | 1258 | CB | SER | 127 | 26.962 | 8.291 | 53.365 | 1.00 | 20.00 |
| ATOM | 1259 | OG | SER | 127 | 28.137 | 8.806 | 52.760 | 1.00 | 20.00 |
| ATOM | 1261 | C | SER | 127 | 27.798 | 5.986 | 53.302 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1262 | O | SER | 127 | 28.995 | 5.712 | 53.212 | 1.00 | 20.00 |
| ATOM | 1263 | N | ASN | 128 | 26.840 | 5.341 | 52.604 | 1.00 | 20.00 |
| ATOM | 1265 | CA | ASN | 128 | 27.126 | 4.347 | 51.610 | 1.00 | 20.00 |
| OM | 1266 | CB | ASN | 128 | 27.619 | 4.946 | 50.280 | 1.00 | 20.00 |
| ATOM | 1267 | CG | ASN | 128 | 26.461 | 5.697 | 49.637 | 1.00 | 20.00 |
| ATOM | 1268 | OD1 | ASN | 128 | 25.444 | 5.108 | 49.275 | 1.00 | 20.00 |
| ATOM | 1269 | ND2 | ASN | 128 | 26.617 | 7.041 | 49.494 | 1.00 | 20.00 |
| ATOM | 1272 | C | ASN | 128 | 28.134 | 3.339 | 52.055 | 1.00 | 20.00 |
| ATOM | 1273 | O | ASN | 128 | 29.252 | 3.306 | 51.542 | 1.00 | 20.00 |
| ATOM | 1274 | N | ASN | 129 | 27.778 | 2.502 | 53.050 | 1.00 | 20.00 |
| ATOM | 1276 | CA | ASN | 129 | 28.702 | 1.470 | 53.428 | 1.00 | 20.00 |
| ATOM | 1277 | CB | ASN | 129 | 29.436 | 1.800 | 54.735 | 1.00 | 20.00 |
| ATOM | 1278 | CG | ASN | 129 | 30.295 | 3.030 | 54.482 | 1.00 | 20.00 |
| ATOM | 1279 | OD1 | ASN | 129 | 31.229 | 2.993 | 53.682 | 1.00 | 20.00 |
| ATOM | 1280 | ND2 | ASN | 129 | 29.965 | 4.156 | 55.170 | 1.00 | 20.00 |
| ATOM | 1283 | C | ASN | 129 | 27.923 | 0.211 | 53.673 | 1.00 | 20.00 |
| ATOM | 1284 | O | ASN | 129 | 27.696 | -0.162 | 54.821 | 1.00 | 20.00 |
| ATOM | 1285 | N | PRO | 130 | 27.598 | -0.495 | 52.620 | 1.00 | 20.00 |
| ATOM | 1286 | CD | PRO | 130 | 28.347 | -0.415 | 51.380 | 1.00 | 20.00 |
| ATOM | 1287 | CA | PRO | 130 | 26.725 | -1.646 | 52.666 | 1.00 | 20.00 |
| ATOM | 1288 | CB | PRO | 130 | 26.874 | -2.340 | 51.311 | 1.00 | 20.00 |
| ATOM | 1289 | CG | PRO | 130 | 27.546 | -1.292 | 50.404 | 1.00 | 20.00 |
| ATOM | 1290 | C | PRO | 130 | 27.007 | -2.592 | 53.801 | 1.00 | 20.00 |
| ATOM | 1291 | O | PRO | 130 | 26.073 | -2.963 | 54.510 | 1.00 | 20.00 |
| ATOM | 1292 | N | ALA | 131 | 28.280 | -2.993 | 53.967 | 1.00 | 20.00 |
| ATOM | 1294 | CA | ALA | 131 | 28.763 | -3.910 | 54.962 | 1.00 | 20.00 |
| ATOM | 1295 | CB | ALA | 131 | 30.131 | -4.505 | 54.587 | 1.00 | 20.00 |
| ATOM | 1296 | C | ALA | 131 | 28.907 | -3.352 | 56.350 | 1.00 | 20.00 |
| ATOM | 1297 | O | ALA | 131 | 28.971 | -4.114 | 57.312 | 1.00 | 20.00 |
| ATOM | 1298 | N | LEU | 132 | 29.031 | -2.020 | 56.492 | 1.00 | 20.00 |
| ATOM | 1300 | CA | LEU | 132 | 29.337 | -1.428 | 57.767 | 1.00 | 20.00 |
| ATOM | 1301 | CB | LEU | 132 | 29.400 | 0.108 | 57.704 | 1.00 | 20.00 |
| ATOM | 1302 | CG | LEU | 132 | 29.742 | 0.793 | 59.038 | 1.00 | 20.00 |
| ATOM | 1303 | CD1 | LEU | 132 | 31.129 | 0.382 | 59.549 | 1.00 | 20.00 |
| ATOM | 1304 | CD2 | LEU | 132 | 29.586 | 2.318 | 58.928 | 1.00 | 20.00 |
| ATOM | 1305 | C | LEU | 132 | 28.388 | -1.818 | 58.852 | 1.00 | 20.00 |
| ATOM | 1306 | O | LEU | 132 | 27.174 | -1.653 | 58.743 | 1.00 | 20.00 |
| ATOM | 1307 | N | CYS | 133 | 28.965 | -2.335 | 59.955 | 1.00 | 20.00 |
| ATOM | 1309 | CA | CYS | 133 | 28.236 | -2.785 | 61.096 | 1.00 | 20.00 |
| ATOM | 1310 | CB | CYS | 133 | 28.392 | -4.290 | 61.352 | 1.00 | 20.00 |
| ATOM | 1311 | SG | CYS | 133 | 27.437 | -5.281 | 60.176 | 1.00 | 20.00 |
| ATOM | 1312 | C | CYS | 133 | 28.804 | -2.090 | 62.292 | 1.00 | 20.00 |
| ATOM | 1313 | O | CYS | 133 | 29.656 | -1.214 | 62.167 | 1.00 | 20.00 |
| ATOM | 1314 | N | ASN | 134 | 28.310 | -2.460 | 63.488 | 1.00 | 20.00 |
| ATOM | 1316 | CA | ASN | 134 | 28.773 | -1.887 | 64.715 | 1.00 | 20.00 |
| ATOM | 1317 | CB | ASN | 134 | 30.193 | -2.332 | 65.107 | 1.00 | 20.00 |
| ATOM | 1318 | CG | ASN | 134 | 30.101 | -3.784 | 65.561 | 1.00 | 20.00 |
| ATOM | 1319 | OD1 | ASN | 134 | 30.893 | -4.632 | 65.156 | 1.00 | 20.00 |
| ATOM | 1320 | ND2 | ASN | 134 | 29.102 | -4.078 | 66.436 | 1.00 | 20.00 |
| ATOM | 1323 | C | ASN | 134 | 28.729 | -0.397 | 64.609 | 1.00 | 20.00 |
| ATOM | 1324 | O | ASN | 134 | 29.653 | 0.292 | 65.040 | 1.00 | 20.00 |
| ATOM | 1325 | N | VAL | 135 | 27.731 | 0.107 | 63.854 | 1.00 | 20.00 |
| ATOM | 1327 | CA | VAL | 135 | 27.391 | 1.500 | 63.755 | 1.00 | 20.00 |
| ATOM | 1328 | CB | VAL | 135 | 26.828 | 1.846 | 62.408 | 1.00 | 20.00 |
| ATOM | 1329 | CG1 | VAL | 135 | 27.912 | 1.585 | 61.349 | 1.00 | 20.00 |
| ATOM | 1330 | CG2 | VAL | 135 | 25.538 | 1.036 | 62.190 | 1.00 | 20.00 |
| ATOM | 1331 | C | VAL | 135 | 26.393 | 1.959 | 64.782 | 1.00 | 20.00 |
| ATOM | 1332 | O | VAL | 135 | 26.512 | 3.040 | 65.353 | 1.00 | 20.00 |
| ATOM | 1333 | N | GLU | 136 | 25.349 | 1.136 | 65.009 | 1.00 | 20.00 |
| ATOM | 1335 | CA | GLU | 136 | 24.252 | 1.436 | 65.892 | 1.00 | 20.00 |
| ATOM | 1336 | CB | GLU | 136 | 23.078 | 0.452 | 65.745 | 1.00 | 20.00 |
| ATOM | 1337 | CG | GLU | 136 | 21.911 | 0.768 | 66.680 | 1.00 | 20.00 |
| ATOM | 1338 | CD | GLU | 136 | 21.210 | 2.009 | 66.147 | 1.00 | 20.00 |
| ATOM | 1339 | OE1 | GLU | 136 | 20.551 | 1.899 | 65.079 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1340 | OE2 | GLU | 136 | 21.327 | 3.082 | 66.798 | 1.00 | 20.00 |
| ATOM | 1341 | C | GLU | 136 | 24.708 | 1.359 | 67.305 | 1.00 | 20.00 |
| ATOM | 1342 | O | GLU | 136 | 24.139 | 1.986 | 68.196 | 1.00 | 20.00 |
| ATOM | 1343 | N | SER | 137 | 25.749 | 0.542 | 67.513 | 1.00 | 20.00 |
| ATOM | 1345 | CA | SER | 137 | 26.349 | 0.181 | 68.762 | 1.00 | 20.00 |
| ATOM | 1346 | CB | SER | 137 | 27.419 | -0.903 | 68.574 | 1.00 | 20.00 |
| ATOM | 1347 | OG | SER | 137 | 26.854 | -2.020 | 67.907 | 1.00 | 20.00 |
| ATOM | 1349 | C | SER | 137 | 27.023 | 1.314 | 69.462 | 1.00 | 20.00 |
| ATOM | 1350 | O | SER | 137 | 27.244 | 1.223 | 70.667 | 1.00 | 20.00 |
| ATOM | 1351 | N | ILE | 138 | 27.452 | 2.377 | 68.753 | 1.00 | 20.00 |
| ATOM | 1353 | CA | ILE | 138 | 28.131 | 3.385 | 69.515 | 1.00 | 20.00 |
| ATOM | 1354 | CB | ILE | 138 | 29.429 | 3.894 | 68.940 | 1.00 | 20.00 |
| ATOM | 1355 | CG2 | ILE | 138 | 30.414 | 2.715 | 68.934 | 1.00 | 20.00 |
| ATOM | 1356 | CG1 | ILE | 138 | 29.257 | 4.560 | 67.568 | 1.00 | 20.00 |
| ATOM | 1357 | CD1 | ILE | 138 | 28.957 | 3.567 | 66.454 | 1.00 | 20.00 |
| ATOM | 1358 | C | ILE | 138 | 27.294 | 4.575 | 69.845 | 1.00 | 20.00 |
| ATOM | 1359 | O | ILE | 138 | 26.422 | 4.989 | 69.082 | 1.00 | 20.00 |
| ATOM | 1360 | N | GLN | 139 | 27.544 | 5.144 | 71.044 | 1.00 | 20.00 |
| ATOM | 1362 | CA | GLN | 139 | 26.824 | 6.306 | 71.473 | 1.00 | 20.00 |
| ATOM | 1363 | CB | GLN | 139 | 26.612 | 6.369 | 72.996 | 1.00 | 20.00 |
| ATOM | 1364 | CG | GLN | 139 | 25.723 | 5.254 | 73.550 | 1.00 | 20.00 |
| ATOM | 1365 | CD | GLN | 139 | 25.608 | 5.455 | 75.055 | 1.00 | 20.00 |
| ATOM | 1366 | OE1 | GLN | 139 | 26.228 | 6.352 | 75.625 | 1.00 | 20.00 |
| ATOM | 1367 | NE2 | GLN | 139 | 24.789 | 4.599 | 75.721 | 1.00 | 20.00 |
| ATOM | 1370 | C | GLN | 139 | 27.653 | 7.494 | 71.108 | 1.00 | 20.00 |
| ATOM | 1371 | O | GLN | 139 | 28.533 | 7.915 | 71.854 | 1.00 | 20.00 |
| ATOM | 1372 | N | TRP | 140 | 27.351 | 8.092 | 69.948 | 1.00 | 20.00 |
| ATOM | 1374 | CA | TRP | 140 | 28.071 | 9.224 | 69.450 | 1.00 | 20.00 |
| ATOM | 1375 | CB | TRP | 140 | 27.692 | 9.605 | 68.010 | 1.00 | 20.00 |
| ATOM | 1376 | CG | TRP | 140 | 28.076 | 8.535 | 67.013 | 1.00 | 20.00 |
| ATOM | 1377 | CD2 | TRP | 140 | 29.428 | 8.220 | 66.635 | 1.00 | 20.00 |
| ATOM | 1378 | CE2 | TRP | 140 | 29.372 | 7.119 | 65.780 | 1.00 | 20.00 |
| ATOM | 1379 | CE3 | TRP | 140 | 30.620 | 8.790 | 66.980 | 1.00 | 20.00 |
| ATOM | 1380 | CD1 | TRP | 140 | 27.281 | 7.613 | 66.398 | 1.00 | 20.00 |
| ATOM | 1381 | NE1 | TRP | 140 | 28.048 | 6.762 | 65.638 | 1.00 | 20.00 |
| ATOM | 1383 | CZ2 | TRP | 140 | 30.508 | 6.574 | 65.251 | 1.00 | 20.00 |
| ATOM | 1384 | CZ3 | TRP | 140 | 31.763 | 8.237 | 66.445 | 1.00 | 20.00 |
| ATOM | 1385 | CH2 | TRP | 140 | 31.709 | 7.152 | 65.595 | 1.00 | 20.00 |
| ATOM | 1386 | C | TRP | 140 | 27.801 | 10.373 | 70.359 | 1.00 | 20.00 |
| ATOM | 1387 | O | TRP | 140 | 28.476 | 11.394 | 70.301 | 1.00 | 20.00 |
| ATOM | 1388 | N | ARG | 141 | 26.754 | 10.253 | 71.190 | 1.00 | 20.00 |
| ATOM | 1390 | CA | ARG | 141 | 26.397 | 11.300 | 72.099 | 1.00 | 20.00 |
| ATOM | 1391 | CB | ARG | 141 | 25.226 | 10.879 | 73.005 | 1.00 | 20.00 |
| ATOM | 1392 | CG | ARG | 141 | 24.596 | 12.002 | 73.831 | 1.00 | 20.00 |
| ATOM | 1393 | CD | ARG | 141 | 23.535 | 11.481 | 74.804 | 1.00 | 20.00 |
| ATOM | 1394 | NE | ARG | 141 | 22.804 | 12.651 | 75.364 | 1.00 | 20.00 |
| ATOM | 1396 | CZ | ARG | 141 | 21.689 | 13.118 | 74.730 | 1.00 | 20.00 |
| ATOM | 1397 | NH1 | ARG | 141 | 21.013 | 14.190 | 75.237 | 1.00 | 20.00 |
| ATOM | 1400 | NH2 | ARG | 141 | 21.246 | 12.509 | 73.591 | 1.00 | 20.00 |
| ATOM | 1403 | C | ARG | 141 | 27.568 | 11.603 | 72.983 | 1.00 | 20.00 |
| ATOM | 1404 | O | ARG | 141 | 27.850 | 12.769 | 73.253 | 1.00 | 20.00 |
| ATOM | 1405 | N | ASP | 142 | 28.270 | 10.571 | 73.493 | 1.00 | 20.00 |
| ATOM | 1407 | CA | ASP | 142 | 29.398 | 10.884 | 74.323 | 1.00 | 20.00 |
| ATOM | 1408 | CB | ASP | 142 | 29.869 | 9.726 | 75.243 | 1.00 | 20.00 |
| ATOM | 1409 | CG | ASP | 142 | 30.337 | 8.470 | 74.513 | 1.00 | 20.00 |
| ATOM | 1410 | OD1 | ASP | 142 | 30.547 | 8.500 | 73.274 | 1.00 | 20.00 |
| ATOM | 1411 | OD2 | ASP | 142 | 30.493 | 7.437 | 75.218 | 1.00 | 20.00 |
| ATOM | 1412 | C | ASP | 142 | 30.543 | 11.452 | 73.533 | 1.00 | 20.00 |
| ATOM | 1413 | O | ASP | 142 | 31.222 | 12.373 | 73.987 | 1.00 | 20.00 |
| ATOM | 1414 | N | ILE | 143 | 30.787 | 10.913 | 72.324 | 1.00 | 20.00 |
| ATOM | 1416 | CA | ILE | 143 | 31.880 | 11.333 | 71.493 | 1.00 | 20.00 |
| ATOM | 1417 | CB | ILE | 143 | 32.102 | 10.348 | 70.369 | 1.00 | 20.00 |
| ATOM | 1418 | CG2 | ILE | 143 | 30.926 | 10.462 | 69.391 | 1.00 | 20.00 |
| ATOM | 1419 | CG1 | ILE | 143 | 33.460 | 10.541 | 69.684 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1420 | CD1 | ILE | 143 | 33.543 | 11.814 | 68.850 | 1.00 | 20.00 |
| ATOM | 1421 | C | ILE | 143 | 31.688 | 12.725 | 70.950 | 1.00 | 20.00 |
| ATOM | 1422 | O | ILE | 143 | 32.602 | 13.546 | 70.998 | 1.00 | 20.00 |
| OM | 1423 | N | VAL | 144 | 30.480 | 13.041 | 70.442 | 1.00 | 20.00 |
| ATOM | 1425 | CA | VAL | 144 | 30.207 | 14.324 | 69.854 | 1.00 | 20.00 |
| ATOM | 1426 | CB | VAL | 144 | 29.753 | 14.239 | 68.426 | 1.00 | 20.00 |
| ATOM | 1427 | CG1 | VAL | 144 | 30.892 | 13.642 | 67.582 | 1.00 | 20.00 |
| ATOM | 1428 | CG2 | VAL | 144 | 28.449 | 13.425 | 68.377 | 1.00 | 20.00 |
| ATOM | 1429 | C | VAL | 144 | 29.090 | 14.942 | 70.630 | 1.00 | 20.00 |
| ATOM | 1430 | O | VAL | 144 | 28.288 | 14.241 | 71.240 | 1.00 | 20.00 |
| ATOM | 1431 | N | SER | 145 | 29.004 | 16.285 | 70.626 | 1.00 | 20.00 |
| ATOM | 1433 | CA | SER | 145 | 27.993 | 16.945 | 71.401 | 1.00 | 20.00 |
| ATOM | 1434 | CB | SER | 145 | 27.967 | 18.470 | 71.217 | 1.00 | 20.00 |
| ATOM | 1435 | OG | SER | 145 | 29.188 | 19.039 | 71.669 | 1.00 | 20.00 |
| ATOM | 1437 | C | SER | 145 | 26.640 | 16.424 | 71.040 | 1.00 | 20.00 |
| ATOM | 1438 | O | SER | 145 | 26.434 | 15.869 | 69.963 | 1.00 | 20.00 |
| ATOM | 1439 | N | SER | 146 | 25.678 | 16.577 | 71.968 | 1.00 | 40.00 |
| ATOM | 1441 | CA | SER | 146 | 24.344 | 16.120 | 71.722 | 1.00 | 40.00 |
| ATOM | 1442 | CB | SER | 146 | 23.417 | 16.297 | 72.935 | 1.00 | 40.00 |
| ATOM | 1443 | OG | SER | 146 | 23.868 | 15.487 | 74.011 | 1.00 | 40.00 |
| ATOM | 1445 | C | SER | 146 | 23.801 | 16.949 | 70.609 | 1.00 | 40.00 |
| ATOM | 1446 | O | SER | 146 | 23.167 | 16.436 | 69.688 | 1.00 | 40.00 |
| ATOM | 1447 | N | ASP | 147 | 24.059 | 18.268 | 70.664 | 1.00 | 40.00 |
| ATOM | 1449 | CA | ASP | 147 | 23.578 | 19.139 | 69.638 | 1.00 | 40.00 |
| ATOM | 1450 | CB | ASP | 147 | 24.004 | 20.603 | 69.840 | 1.00 | 40.00 |
| ATOM | 1451 | CG | ASP | 147 | 23.299 | 21.444 | 68.785 | 1.00 | 40.00 |
| ATOM | 1452 | OD1 | ASP | 147 | 22.361 | 20.911 | 68.135 | 1.00 | 40.00 |
| ATOM | 1453 | OD2 | ASP | 147 | 23.693 | 22.629 | 68.613 | 1.00 | 40.00 |
| ATOM | 1454 | C | ASP | 147 | 24.208 | 18.667 | 68.373 | 1.00 | 40.00 |
| ATOM | 1455 | O | ASP | 147 | 23.561 | 18.599 | 67.329 | 1.00 | 40.00 |
| ATOM | 1456 | N | PHE | 148 | 25.502 | 18.307 | 68.448 | 1.00 | 40.00 |
| ATOM | 1458 | CA | PHE | 148 | 26.182 | 17.857 | 67.280 | 1.00 | 40.00 |
| ATOM | 1459 | CB | PHE | 148 | 27.692 | 17.655 | 67.485 | 1.00 | 40.00 |
| ATOM | 1460 | CG | PHE | 148 | 28.305 | 19.013 | 67.455 | 1.00 | 40.00 |
| ATOM | 1461 | CD1 | PHE | 148 | 28.659 | 19.580 | 66.253 | 1.00 | 40.00 |
| ATOM | 1462 | CD2 | PHE | 148 | 28.480 | 19.742 | 68.608 | 1.00 | 40.00 |
| ATOM | 1463 | CE1 | PHE | 148 | 29.191 | 20.846 | 66.203 | 1.00 | 40.00 |
| ATOM | 1464 | CE2 | PHE | 148 | 29.014 | 21.009 | 68.565 | 1.00 | 40.00 |
| ATOM | 1465 | CZ | PHE | 148 | 29.373 | 21.564 | 67.361 | 1.00 | 40.00 |
| ATOM | 1466 | C | PHE | 148 | 25.596 | 16.582 | 66.770 | 1.00 | 40.00 |
| ATOM | 1467 | O | PHE | 148 | 25.551 | 16.361 | 65.562 | 1.00 | 40.00 |
| ATOM | 1468 | N | LEU | 149 | 25.100 | 15.717 | 67.672 | 1.00 | 40.00 |
| ATOM | 1470 | CA | LEU | 149 | 24.608 | 14.440 | 67.240 | 1.00 | 40.00 |
| ATOM | 1471 | CB | LEU | 149 | 24.069 | 13.569 | 68.387 | 1.00 | 40.00 |
| ATOM | 1472 | CG | LEU | 149 | 23.546 | 12.205 | 67.900 | 1.00 | 40.00 |
| ATOM | 1473 | CD1 | LEU | 149 | 24.670 | 11.377 | 67.254 | 1.00 | 40.00 |
| ATOM | 1474 | CD2 | LEU | 149 | 22.825 | 11.446 | 69.023 | 1.00 | 40.00 |
| ATOM | 1475 | C | LEU | 149 | 23.505 | 14.619 | 66.249 | 1.00 | 40.00 |
| ATOM | 1476 | O | LEU | 149 | 23.379 | 13.843 | 65.303 | 1.00 | 40.00 |
| ATOM | 1477 | N | SER | 150 | 22.675 | 15.664 | 66.425 | 1.00 | 40.00 |
| ATOM | 1479 | CA | SER | 150 | 21.578 | 15.868 | 65.523 | 1.00 | 40.00 |
| ATOM | 1480 | CB | SER | 150 | 20.763 | 17.128 | 65.857 | 1.00 | 40.00 |
| ATOM | 1481 | OG | SER | 150 | 21.564 | 18.288 | 65.698 | 1.00 | 40.00 |
| ATOM | 1483 | C | SER | 150 | 22.114 | 16.030 | 64.135 | 1.00 | 40.00 |
| ATOM | 1484 | O | SER | 150 | 21.501 | 15.583 | 63.167 | 1.00 | 40.00 |
| ATOM | 1485 | N | ASN | 151 | 23.286 | 16.678 | 64.015 | 1.00 | 40.00 |
| ATOM | 1487 | CA | ASN | 151 | 23.919 | 16.977 | 62.762 | 1.00 | 40.00 |
| ATOM | 1488 | CB | ASN | 151 | 25.177 | 17.844 | 62.937 | 1.00 | 40.00 |
| ATOM | 1489 | CG | ASN | 151 | 24.741 | 19.195 | 63.487 | 1.00 | 40.00 |
| ATOM | 1490 | OD1 | ASN | 151 | 23.656 | 19.688 | 63.180 | 1.00 | 40.00 |
| ATOM | 1491 | ND2 | ASN | 151 | 25.612 | 19.813 | 64.329 | 1.00 | 40.00 |
| ATOM | 1494 | C | ASN | 151 | 24.341 | 15.743 | 62.019 | 1.00 | 40.00 |
| ATOM | 1495 | O | ASN | 151 | 24.380 | 15.740 | 60.790 | 1.00 | 40.00 |
| ATOM | 1496 | N | MET | 152 | 24.686 | 14.664 | 62.747 | 1.00 | 40.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1498 | CA | MET | 152 | 25.193 | 13.461 | 62.147 | 1.00 | 40.00 |
| ATOM | 1499 | CB | MET | 152 | 25.308 | 12.309 | 63.162 | 1.00 | 40.00 |
| ATOM | 1500 | CG | MET | 152 | 25.897 | 11.013 | 62.602 | 1.00 | 40.00 |
| ATOM | 1501 | SD | MET | 152 | 26.051 | 9.686 | 63.835 | 1.00 | 40.00 |
| ATOM | 1502 | CE | MET | 152 | 26.754 | 8.460 | 62.697 | 1.00 | 40.00 |
| ATOM | 1503 | C | MET | 152 | 24.326 | 13.011 | 61.016 | 1.00 | 40.00 |
| ATOM | 1504 | O | MET | 152 | 23.101 | 13.009 | 61.115 | 1.00 | 40.00 |
| ATOM | 1505 | N | SER | 153 | 24.967 | 12.636 | 59.887 | 1.00 | 40.00 |
| ATOM | 1507 | CA | SER | 153 | 24.220 | 12.200 | 58.745 | 1.00 | 40.00 |
| ATOM | 1508 | CB | SER | 153 | 24.502 | 13.023 | 57.473 | 1.00 | 40.00 |
| ATOM | 1509 | OG | SER | 153 | 23.728 | 12.530 | 56.390 | 1.00 | 40.00 |
| ATOM | 1511 | C | SER | 153 | 24.586 | 10.788 | 58.441 | 1.00 | 40.00 |
| ATOM | 1512 | O | SER | 153 | 25.725 | 10.484 | 58.086 | 1.00 | 40.00 |
| ATOM | 1513 | N | MET | 154 | 23.612 | 9.872 | 58.577 | 1.00 | 40.00 |
| ATOM | 1515 | CA | MET | 154 | 23.874 | 8.509 | 58.242 | 1.00 | 40.00 |
| ATOM | 1516 | CB | MET | 154 | 23.599 | 7.514 | 59.384 | 1.00 | 40.00 |
| ATOM | 1517 | CG | MET | 154 | 23.890 | 6.064 | 58.993 | 1.00 | 40.00 |
| ATOM | 1518 | SD | MET | 154 | 23.588 | 4.841 | 60.306 | 1.00 | 40.00 |
| ATOM | 1519 | CE | MET | 154 | 25.146 | 5.148 | 61.184 | 1.00 | 40.00 |
| ATOM | 1520 | C | MET | 154 | 22.942 | 8.173 | 57.137 | 1.00 | 40.00 |
| ATOM | 1521 | O | MET | 154 | 21.741 | 8.426 | 57.230 | 1.00 | 40.00 |
| ATOM | 1522 | N | ASP | 155 | 23.463 | 7.600 | 56.040 | 1.00 | 40.00 |
| ATOM | 1524 | CA | ASP | 155 | 22.536 | 7.273 | 55.010 | 1.00 | 40.00 |
| ATOM | 1525 | CB | ASP | 155 | 22.995 | 7.565 | 53.563 | 1.00 | 40.00 |
| ATOM | 1526 | CG | ASP | 155 | 24.145 | 6.657 | 53.156 | 1.00 | 40.00 |
| ATOM | 1527 | OD1 | ASP | 155 | 24.405 | 6.563 | 51.927 | 1.00 | 40.00 |
| ATOM | 1528 | OD2 | ASP | 155 | 24.773 | 6.038 | 54.051 | 1.00 | 40.00 |
| ATOM | 1529 | C | ASP | 155 | 22.264 | 5.822 | 55.133 | 1.00 | 40.00 |
| ATOM | 1530 | O | ASP | 155 | 23.085 | 5.059 | 55.646 | 1.00 | 40.00 |
| ATOM | 1531 | N | PHE | 156 | 21.080 | 5.440 | 54.628 | 1.00 | 40.00 |
| ATOM | 1533 | CA | PHE | 156 | 20.544 | 4.117 | 54.646 | 1.00 | 40.00 |
| ATOM | 1534 | CB | PHE | 156 | 19.243 | 4.042 | 53.826 | 1.00 | 40.00 |
| ATOM | 1535 | CG | PHE | 156 | 18.768 | 2.632 | 53.757 | 1.00 | 40.00 |
| ATOM | 1536 | CD1 | PHE | 156 | 18.067 | 2.069 | 54.797 | 1.00 | 40.00 |
| ATOM | 1537 | CD2 | PHE | 156 | 18.934 | 1.913 | 52.596 | 1.00 | 40.00 |
| ATOM | 1538 | CE1 | PHE | 156 | 17.563 | 0.794 | 54.688 | 1.00 | 40.00 |
| ATOM | 1539 | CE2 | PHE | 156 | 18.435 | 0.637 | 52.482 | 1.00 | 40.00 |
| ATOM | 1540 | CZ | PHE | 156 | 17.747 | 0.076 | 53.531 | 1.00 | 40.00 |
| ATOM | 1541 | C | PHE | 156 | 21.540 | 3.207 | 54.022 | 1.00 | 40.00 |
| ATOM | 1542 | O | PHE | 156 | 21.535 | 2.002 | 54.267 | 1.00 | 40.00 |
| ATOM | 1543 | N | GLN | 157 | 22.447 | 3.768 | 53.207 | 1.00 | 40.00 |
| ATOM | 1545 | CA | GLN | 157 | 23.349 | 2.907 | 52.518 | 1.00 | 40.00 |
| ATOM | 1546 | CB | GLN | 157 | 24.276 | 3.608 | 51.518 | 1.00 | 40.00 |
| ATOM | 1547 | CG | GLN | 157 | 24.984 | 2.599 | 50.609 | 1.00 | 40.00 |
| ATOM | 1548 | CD | GLN | 157 | 23.914 | 1.839 | 49.835 | 1.00 | 40.00 |
| ATOM | 1549 | OE1 | GLN | 157 | 22.728 | 2.158 | 49.910 | 1.00 | 40.00 |
| ATOM | 1550 | NE2 | GLN | 157 | 24.342 | 0.797 | 49.072 | 1.00 | 40.00 |
| ATOM | 1553 | C | GLN | 157 | 24.172 | 2.079 | 53.456 | 1.00 | 40.00 |
| ATOM | 1554 | O | GLN | 157 | 24.886 | 1.187 | 53.008 | 1.00 | 40.00 |
| ATOM | 1555 | N | ASN | 158 | 24.126 | 2.350 | 54.776 | 1.00 | 40.00 |
| ATOM | 1557 | CA | ASN | 158 | 24.867 | 1.507 | 55.675 | 1.00 | 40.00 |
| ATOM | 1558 | CB | ASN | 158 | 25.044 | 2.095 | 57.084 | 1.00 | 40.00 |
| ATOM | 1559 | CG | ASN | 158 | 26.028 | 3.251 | 56.984 | 1.00 | 40.00 |
| ATOM | 1560 | OD1 | ASN | 158 | 26.920 | 3.251 | 56.136 | 1.00 | 40.00 |
| ATOM | 1561 | ND2 | ASN | 158 | 25.869 | 4.264 | 57.877 | 1.00 | 40.00 |
| ATOM | 1564 | C | ASN | 158 | 24.131 | 0.208 | 55.803 | 1.00 | 40.00 |
| ATOM | 1565 | O | ASN | 158 | 23.093 | 0.012 | 55.175 | 1.00 | 40.00 |
| ATOM | 1566 | N | HIS | 159 | 24.671 | -0.732 | 56.607 | 1.00 | 40.00 |
| ATOM | 1568 | CA | HIS | 159 | 24.049 | -2.020 | 56.748 | 1.00 | 40.00 |
| ATOM | 1569 | CB | HIS | 159 | 25.033 | -3.127 | 57.165 | 1.00 | 40.00 |
| ATOM | 1570 | CG | HIS | 159 | 24.457 | -4.507 | 57.054 | 1.00 | 40.00 |
| ATOM | 1571 | CD2 | HIS | 159 | 24.069 | -5.379 | 58.023 | 1.00 | 40.00 |
| ATOM | 1572 | ND1 | HIS | 159 | 24.246 | -5.157 | 55.858 | 1.00 | 40.00 |
| ATOM | 1574 | CE1 | HIS | 159 | 23.740 | -6.379 | 56.160 | 1.00 | 40.00 |

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|-------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1575 | NE2 | HIS | 159 | 23.614 | -6.560 | 57.463 | 1.00 | 40.00 |
| ATOM | 1577 | C | HIS | 159 | 22.963 | -1.954 | 57.779 | 1.00 | 40.00 |
| ATOM | 1578 | O | HIS | 159 | 22.940 | -1.052 | 58.614 | 1.00 | 40.00 |
| OM | 1579 | N | LEU | 160 | 22.020 | -2.922 | 57.735 | 1.00 | 40.00 |
| ...OM | 1581 | CA | LEU | 160 | 20.933 | -2.939 | 58.671 | 1.00 | 40.00 |
| ATOM | 1582 | CB | LEU | 160 | 19.700 | -3.721 | 58.183 | 1.00 | 40.00 |
| ATOM | 1583 | CG | LEU | 160 | 19.036 | -3.116 | 56.933 | 1.00 | 40.00 |
| ATOM | 1584 | CD1 | LEU | 160 | 19.969 | -3.190 | 55.714 | 1.00 | 40.00 |
| ATOM | 1585 | CD2 | LEU | 160 | 17.660 | -3.751 | 56.672 | 1.00 | 40.00 |
| ATOM | 1586 | C | LEU | 160 | 21.396 | -3.580 | 59.941 | 1.00 | 40.00 |
| ATOM | 1587 | O | LEU | 160 | 22.356 | -4.345 | 59.956 | 1.00 | 40.00 |
| ATOM | 1588 | N | GLY | 161 | 20.671 | -3.307 | 61.042 | 1.00 | 40.00 |
| ATOM | 1590 | CA | GLY | 161 | 20.984 | -3.755 | 62.372 | 1.00 | 40.00 |
| ATOM | 1591 | C | GLY | 161 | 21.076 | -5.247 | 62.474 | 1.00 | 40.00 |
| ATOM | 1592 | O | GLY | 161 | 21.366 | -5.783 | 63.542 | 1.00 | 40.00 |
| ATOM | 1593 | N | SER | 162 | 20.837 | -5.955 | 61.359 | 1.00 | 40.00 |
| ATOM | 1595 | CA | SER | 162 | 20.887 | -7.388 | 61.308 | 1.00 | 40.00 |
| ATOM | 1596 | CB | SER | 162 | 20.644 | -7.945 | 59.896 | 1.00 | 40.00 |
| ATOM | 1597 | OG | SER | 162 | 20.708 | -9.364 | 59.915 | 1.00 | 40.00 |
| ATOM | 1599 | C | SER | 162 | 22.260 | -7.815 | 61.734 | 1.00 | 40.00 |
| ATOM | 1600 | O | SER | 162 | 22.481 | -8.959 | 62.127 | 1.00 | 40.00 |
| ATOM | 1601 | N | CYS | 163 | 23.229 | -6.888 | 61.661 | 1.00 | 40.00 |
| ATOM | 1603 | CA | CYS | 163 | 24.610 | -7.156 | 61.943 | 1.00 | 40.00 |
| ATOM | 1604 | CB | CYS | 163 | 25.371 | -5.859 | 62.222 | 1.00 | 40.00 |
| ATOM | 1605 | SG | CYS | 163 | 25.554 | -4.822 | 60.750 | 1.00 | 40.00 |
| ATOM | 1606 | C | CYS | 163 | 24.886 | -8.059 | 63.119 | 1.00 | 40.00 |
| ATOM | 1607 | O | CYS | 163 | 25.394 | -9.158 | 62.913 | 1.00 | 40.00 |
| ATOM | 1608 | N | GLN | 164 | 24.587 | -7.659 | 64.380 | 1.00 | 40.00 |
| ATOM | 1610 | CA | GLN | 164 | 24.973 | -8.554 | 65.450 | 1.00 | 40.00 |
| ATOM | 1611 | CB | GLN | 164 | 26.484 | -8.826 | 65.471 | 1.00 | 40.00 |
| ATOM | 1612 | CG | GLN | 164 | 27.309 | -7.566 | 65.753 | 1.00 | 40.00 |
| ATOM | 1613 | CD | GLN | 164 | 28.783 | -7.943 | 65.755 | 1.00 | 40.00 |
| ATOM | 1614 | OE1 | GLN | 164 | 29.153 | -9.070 | 65.434 | 1.00 | 40.00 |
| ATOM | 1615 | NE2 | GLN | 164 | 29.654 | -6.968 | 66.131 | 1.00 | 40.00 |
| ATOM | 1618 | C | GLN | 164 | 24.637 | -8.001 | 66.809 | 1.00 | 40.00 |
| ATOM | 1619 | O | GLN | 164 | 23.602 | -7.363 | 66.996 | 1.00 | 40.00 |
| ATOM | 1620 | N | LYS | 165 | 25.511 | -8.286 | 67.811 | 1.00 | 40.00 |
| ATOM | 1622 | CA | LYS | 165 | 25.328 | -7.828 | 69.167 | 1.00 | 40.00 |
| ATOM | 1623 | CB | LYS | 165 | 24.424 | -8.751 | 70.000 | 1.00 | 40.00 |
| ATOM | 1624 | CG | LYS | 165 | 22.993 | -8.779 | 69.455 | 1.00 | 40.00 |
| ATOM | 1625 | CD | LYS | 165 | 22.111 | -9.891 | 70.021 | 1.00 | 40.00 |
| ATOM | 1626 | CE | LYS | 165 | 20.752 | -9.994 | 69.322 | 1.00 | 40.00 |
| ATOM | 1627 | NZ | LYS | 165 | 20.004 | -8.724 | 69.468 | 1.00 | 40.00 |
| ATOM | 1631 | C | LYS | 165 | 26.668 | -7.709 | 69.849 | 1.00 | 40.00 |
| ATOM | 1632 | O | LYS | 165 | 27.674 | -8.220 | 69.358 | 1.00 | 40.00 |
| ATOM | 1633 | N | CYS | 166 | 26.712 | -7.013 | 71.011 | 1.00 | 20.00 |
| ATOM | 1635 | CA | CYS | 166 | 27.947 | -6.772 | 71.718 | 1.00 | 20.00 |
| ATOM | 1636 | CB | CYS | 166 | 28.006 | -5.409 | 72.445 | 1.00 | 20.00 |
| ATOM | 1637 | SG | CYS | 166 | 27.870 | -3.949 | 71.364 | 1.00 | 20.00 |
| ATOM | 1638 | C | CYS | 166 | 28.175 | -7.810 | 72.772 | 1.00 | 20.00 |
| ATOM | 1639 | O | CYS | 166 | 27.458 | -8.806 | 72.858 | 1.00 | 20.00 |
| ATOM | 1640 | N | ASP | 167 | 29.221 | -7.588 | 73.598 | 1.00 | 20.00 |
| ATOM | 1642 | CA | ASP | 167 | 29.568 | -8.493 | 74.655 | 1.00 | 20.00 |
| ATOM | 1643 | CB | ASP | 167 | 31.034 | -8.383 | 75.105 | 1.00 | 20.00 |
| ATOM | 1644 | CG | ASP | 167 | 31.911 | -8.872 | 73.962 | 1.00 | 20.00 |
| ATOM | 1645 | OD1 | ASP | 167 | 31.345 | -9.325 | 72.932 | 1.00 | 20.00 |
| ATOM | 1646 | OD2 | ASP | 167 | 33.160 | -8.804 | 74.107 | 1.00 | 20.00 |
| ATOM | 1647 | C | ASP | 167 | 28.717 | -8.188 | 75.845 | 1.00 | 20.00 |
| ATOM | 1648 | O | ASP | 167 | 28.188 | -7.087 | 75.987 | 1.00 | 20.00 |
| ATOM | 1649 | N | PRO | 168 | 28.553 | -9.167 | 76.691 | 1.00 | 20.00 |
| ATOM | 1650 | CD | PRO | 168 | 28.483 | -10.545 | 76.233 | 1.00 | 20.00 |
| ATOM | 1651 | CA | PRO | 168 | 27.792 | -8.962 | 77.891 | 1.00 | 20.00 |
| ATOM | 1652 | CB | PRO | 168 | 27.541 | -10.352 | 78.468 | 1.00 | 20.00 |
| ATOM | 1653 | CG | PRO | 168 | 27.548 | -11.259 | 77.224 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1654 | C | PRO | 168 | 28.529 | -8.037 | 78.800 | 1.00 | 20.00 |
| ATOM | 1655 | O | PRO | 168 | 27.901 | -7.408 | 79.651 | 1.00 | 20.00 |
| ATOM | 1656 | N | SER | 169 | 29.863 | -7.961 | 78.653 | 1.00 | 20.00 |
| ATOM | 1658 | CA | SER | 169 | 30.671 | -7.115 | 79.481 | 1.00 | 20.00 |
| ATOM | 1659 | CB | SER | 169 | 32.175 | -7.337 | 79.251 | 1.00 | 20.00 |
| ATOM | 1660 | OG | SER | 169 | 32.929 | -6.474 | 80.089 | 1.00 | 20.00 |
| ATOM | 1662 | C | SER | 169 | 30.385 | -5.681 | 79.188 | 1.00 | 20.00 |
| ATOM | 1663 | O | SER | 169 | 30.266 | -4.860 | 80.096 | 1.00 | 20.00 |
| ATOM | 1664 | N | CYS | 170 | 30.245 | -5.338 | 77.893 | 1.00 | 20.00 |
| ATOM | 1666 | CA | CYS | 170 | 30.047 | -3.970 | 77.527 | 1.00 | 20.00 |
| ATOM | 1667 | CB | CYS | 170 | 29.930 | -3.734 | 76.011 | 1.00 | 20.00 |
| ATOM | 1668 | SG | CYS | 170 | 31.315 | -4.412 | 75.053 | 1.00 | 20.00 |
| ATOM | 1669 | C | CYS | 170 | 28.745 | -3.530 | 78.102 | 1.00 | 20.00 |
| ATOM | 1670 | O | CYS | 170 | 27.974 | -4.316 | 78.647 | 1.00 | 20.00 |
| ATOM | 1671 | N | PRO | 171 | 28.514 | -2.253 | 78.002 | 1.00 | 20.00 |
| ATOM | 1672 | CD | PRO | 171 | 29.596 | -1.292 | 78.150 | 1.00 | 20.00 |
| ATOM | 1673 | CA | PRO | 171 | 27.261 | -1.721 | 78.446 | 1.00 | 20.00 |
| ATOM | 1674 | CB | PRO | 171 | 27.450 | -0.210 | 78.515 | 1.00 | 20.00 |
| ATOM | 1675 | CG | PRO | 171 | 28.955 | -0.053 | 78.798 | 1.00 | 20.00 |
| ATOM | 1676 | C | PRO | 171 | 26.247 | -2.180 | 77.457 | 1.00 | 20.00 |
| ATOM | 1677 | O | PRO | 171 | 26.624 | -2.504 | 76.332 | 1.00 | 20.00 |
| ATOM | 1678 | N | ASN | 172 | 24.962 | -2.223 | 77.846 | 1.00 | 20.00 |
| ATOM | 1680 | CA | ASN | 172 | 23.973 | -2.748 | 76.955 | 1.00 | 20.00 |
| ATOM | 1681 | CB | ASN | 172 | 22.540 | -2.700 | 77.517 | 1.00 | 20.00 |
| ATOM | 1682 | CG | ASN | 172 | 22.449 | -3.681 | 78.675 | 1.00 | 20.00 |
| ATOM | 1683 | OD1 | ASN | 172 | 23.461 | -4.092 | 79.240 | 1.00 | 20.00 |
| ATOM | 1684 | ND2 | ASN | 172 | 21.198 | -4.074 | 79.036 | 1.00 | 20.00 |
| ATOM | 1687 | C | ASN | 172 | 23.961 | -2.023 | 75.651 | 1.00 | 20.00 |
| ATOM | 1688 | O | ASN | 172 | 23.484 | -0.894 | 75.552 | 1.00 | 20.00 |
| ATOM | 1689 | N | GLY | 173 | 24.513 | -2.674 | 74.609 | 1.00 | 20.00 |
| ATOM | 1691 | CA | GLY | 173 | 24.434 | -2.157 | 73.276 | 1.00 | 20.00 |
| ATOM | 1692 | C | GLY | 173 | 25.496 | -1.168 | 72.921 | 1.00 | 20.00 |
| ATOM | 1693 | O | GLY | 173 | 25.466 | -0.616 | 71.822 | 1.00 | 20.00 |
| ATOM | 1694 | N | SER | 174 | 26.471 | -0.895 | 73.807 | 1.00 | 20.00 |
| ATOM | 1696 | CA | SER | 174 | 27.427 | 0.082 | 73.367 | 1.00 | 20.00 |
| ATOM | 1697 | CB | SER | 174 | 27.613 | 1.251 | 74.348 | 1.00 | 20.00 |
| ATOM | 1698 | OG | SER | 174 | 26.414 | 2.007 | 74.427 | 1.00 | 20.00 |
| ATOM | 1700 | C | SER | 174 | 28.770 | -0.540 | 73.156 | 1.00 | 20.00 |
| ATOM | 1701 | O | SER | 174 | 29.426 | -0.961 | 74.108 | 1.00 | 20.00 |
| ATOM | 1702 | N | CYS | 175 | 29.213 | -0.629 | 71.883 | 1.00 | 20.00 |
| ATOM | 1704 | CA | CYS | 175 | 30.524 | -1.156 | 71.631 | 1.00 | 20.00 |
| ATOM | 1705 | CB | CYS | 175 | 30.629 | -2.687 | 71.827 | 1.00 | 20.00 |
| ATOM | 1706 | SG | CYS | 175 | 29.735 | -3.685 | 70.593 | 1.00 | 20.00 |
| ATOM | 1707 | C | CYS | 175 | 30.933 | -0.843 | 70.226 | 1.00 | 20.00 |
| ATOM | 1708 | O | CYS | 175 | 30.096 | -0.687 | 69.339 | 1.00 | 20.00 |
| ATOM | 1709 | N | TRP | 176 | 32.254 | -0.693 | 70.011 | 1.00 | 20.00 |
| ATOM | 1711 | CA | TRP | 176 | 32.809 | -0.427 | 68.715 | 1.00 | 20.00 |
| ATOM | 1712 | CB | TRP | 176 | 34.264 | 0.062 | 68.806 | 1.00 | 20.00 |
| ATOM | 1713 | CG | TRP | 176 | 34.394 | 1.381 | 69.536 | 1.00 | 20.00 |
| ATOM | 1714 | CD2 | TRP | 176 | 34.070 | 2.660 | 68.967 | 1.00 | 20.00 |
| ATOM | 1715 | CE2 | TRP | 176 | 34.267 | 3.619 | 69.961 | 1.00 | 20.00 |
| ATOM | 1716 | CE3 | TRP | 176 | 33.638 | 3.006 | 67.718 | 1.00 | 20.00 |
| ATOM | 1717 | CD1 | TRP | 176 | 34.748 | 1.618 | 70.833 | 1.00 | 20.00 |
| ATOM | 1718 | NE1 | TRP | 176 | 34.689 | 2.966 | 71.100 | 1.00 | 20.00 |
| ATOM | 1720 | CZ2 | TRP | 176 | 34.039 | 4.945 | 69.718 | 1.00 | 20.00 |
| ATOM | 1721 | CZ3 | TRP | 176 | 33.404 | 4.341 | 67.480 | 1.00 | 20.00 |
| ATOM | 1722 | CH2 | TRP | 176 | 33.601 | 5.292 | 68.458 | 1.00 | 20.00 |
| ATOM | 1723 | C | TRP | 176 | 32.767 | -1.662 | 67.868 | 1.00 | 20.00 |
| ATOM | 1724 | O | TRP | 176 | 32.515 | -1.602 | 66.665 | 1.00 | 20.00 |
| ATOM | 1725 | N | GLY | 177 | 33.028 | -2.826 | 68.493 | 1.00 | 20.00 |
| ATOM | 1727 | CA | GLY | 177 | 33.027 | -4.074 | 67.786 | 1.00 | 20.00 |
| ATOM | 1728 | C | GLY | 177 | 32.794 | -5.125 | 68.820 | 1.00 | 20.00 |
| ATOM | 1729 | O | GLY | 177 | 32.595 | -4.818 | 69.994 | 1.00 | 20.00 |
| ATOM | 1730 | N | ALA | 178 | 32.791 | -6.406 | 68.410 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1732 | CA | ALA | 178 | 32.582 | -7.432 | 69.385 | 1.00 | 20.00 |
| ATOM | 1733 | CB | ALA | 178 | 32.153 | -8.780 | 68.782 | 1.00 | 20.00 |
| ATOM | 1734 | C | ALA | 178 | 33.875 | -7.645 | 70.100 | 1.00 | 20.00 |
| OM | 1735 | O | ALA | 178 | 34.887 | -7.982 | 69.487 | 1.00 | 20.00 |
| ATOM | 1736 | N | GLY | 179 | 33.868 | -7.445 | 71.431 | 1.00 | 20.00 |
| ATOM | 1738 | CA | GLY | 179 | 35.059 | -7.639 | 72.203 | 1.00 | 20.00 |
| ATOM | 1739 | C | GLY | 179 | 34.927 | -6.812 | 73.439 | 1.00 | 20.00 |
| ATOM | 1740 | O | GLY | 179 | 34.295 | -5.757 | 73.429 | 1.00 | 20.00 |
| ATOM | 1741 | N | GLU | 180 | 35.529 | -7.282 | 74.546 | 1.00 | 20.00 |
| ATOM | 1743 | CA | GLU | 180 | 35.459 | -6.562 | 75.782 | 1.00 | 20.00 |
| ATOM | 1744 | CB | GLU | 180 | 36.109 | -7.332 | 76.946 | 1.00 | 20.00 |
| ATOM | 1745 | CG | GLU | 180 | 35.881 | -6.693 | 78.317 | 1.00 | 20.00 |
| ATOM | 1746 | CD | GLU | 180 | 36.375 | -7.672 | 79.373 | 1.00 | 20.00 |
| ATOM | 1747 | OE1 | GLU | 180 | 36.831 | -8.780 | 78.984 | 1.00 | 20.00 |
| ATOM | 1748 | OE2 | GLU | 180 | 36.297 | -7.327 | 80.582 | 1.00 | 20.00 |
| ATOM | 1749 | C | GLU | 180 | 36.192 | -5.273 | 75.597 | 1.00 | 20.00 |
| ATOM | 1750 | O | GLU | 180 | 35.742 | -4.217 | 76.036 | 1.00 | 20.00 |
| ATOM | 1751 | N | GLU | 181 | 37.353 | -5.343 | 74.924 | 1.00 | 20.00 |
| ATOM | 1753 | CA | GLU | 181 | 38.158 | -4.188 | 74.662 | 1.00 | 20.00 |
| ATOM | 1754 | CB | GLU | 181 | 39.505 | -4.543 | 74.007 | 1.00 | 20.00 |
| ATOM | 1755 | CG | GLU | 181 | 40.467 | -3.359 | 73.892 | 1.00 | 20.00 |
| ATOM | 1756 | CD | GLU | 181 | 41.744 | -3.859 | 73.231 | 1.00 | 20.00 |
| ATOM | 1757 | OE1 | GLU | 181 | 42.734 | -3.080 | 73.194 | 1.00 | 20.00 |
| ATOM | 1758 | OE2 | GLU | 181 | 41.750 | -5.028 | 72.761 | 1.00 | 20.00 |
| ATOM | 1759 | C | GLU | 181 | 37.399 | -3.309 | 73.724 | 1.00 | 20.00 |
| ATOM | 1760 | O | GLU | 181 | 37.473 | -2.083 | 73.798 | 1.00 | 20.00 |
| ATOM | 1761 | N | ASN | 182 | 36.632 | -3.946 | 72.821 | 1.00 | 20.00 |
| ATOM | 1763 | CA | ASN | 182 | 35.877 | -3.278 | 71.806 | 1.00 | 20.00 |
| ATOM | 1764 | CB | ASN | 182 | 35.133 | -4.250 | 70.876 | 1.00 | 20.00 |
| ATOM | 1765 | CG | ASN | 182 | 36.159 | -4.895 | 69.958 | 1.00 | 20.00 |
| ATOM | 1766 | OD1 | ASN | 182 | 36.626 | -6.006 | 70.202 | 1.00 | 20.00 |
| ATOM | 1767 | ND2 | ASN | 182 | 36.519 | -4.174 | 68.863 | 1.00 | 20.00 |
| ATOM | 1770 | C | ASN | 182 | 34.862 | -2.373 | 72.420 | 1.00 | 20.00 |
| ATOM | 1771 | O | ASN | 182 | 34.486 | -1.378 | 71.802 | 1.00 | 20.00 |
| ATOM | 1772 | N | CYS | 183 | 34.385 | -2.721 | 73.636 | 1.00 | 20.00 |
| ATOM | 1774 | CA | CYS | 183 | 33.391 | -1.959 | 74.344 | 1.00 | 20.00 |
| ATOM | 1775 | CB | CYS | 183 | 33.302 | -2.281 | 75.846 | 1.00 | 20.00 |
| ATOM | 1776 | SG | CYS | 183 | 32.927 | -4.017 | 76.211 | 1.00 | 20.00 |
| ATOM | 1777 | C | CYS | 183 | 33.734 | -0.519 | 74.270 | 1.00 | 20.00 |
| ATOM | 1778 | O | CYS | 183 | 34.905 | -0.150 | 74.228 | 1.00 | 20.00 |
| ATOM | 1779 | N | GLN | 184 | 32.705 | 0.341 | 74.212 | 1.00 | 60.00 |
| ATOM | 1781 | CA | GLN | 184 | 33.052 | 1.720 | 74.177 | 1.00 | 60.00 |
| ATOM | 1782 | CB | GLN | 184 | 31.868 | 2.667 | 73.922 | 1.00 | 60.00 |
| ATOM | 1783 | CG | GLN | 184 | 32.280 | 4.138 | 73.840 | 1.00 | 60.00 |
| ATOM | 1784 | CD | GLN | 184 | 31.040 | 4.956 | 73.509 | 1.00 | 60.00 |
| ATOM | 1785 | OE1 | GLN | 184 | 30.966 | 5.609 | 72.468 | 1.00 | 60.00 |
| ATOM | 1786 | NE2 | GLN | 184 | 30.032 | 4.919 | 74.420 | 1.00 | 60.00 |
| ATOM | 1789 | C | GLN | 184 | 33.564 | 1.942 | 75.554 | 1.00 | 60.00 |
| ATOM | 1790 | O | GLN | 184 | 32.819 | 1.836 | 76.528 | 1.00 | 60.00 |
| ATOM | 1791 | N | LYS | 185 | 34.872 | 2.229 | 75.669 | 1.00 | 60.00 |
| ATOM | 1793 | CA | LYS | 185 | 35.432 | 2.376 | 76.975 | 1.00 | 60.00 |
| ATOM | 1794 | CB | LYS | 185 | 36.970 | 2.443 | 77.002 | 1.00 | 60.00 |
| ATOM | 1795 | CG | LYS | 185 | 37.567 | 3.707 | 76.384 | 1.00 | 60.00 |
| ATOM | 1796 | CD | LYS | 185 | 39.064 | 3.845 | 76.667 | 1.00 | 60.00 |
| ATOM | 1797 | CE | LYS | 185 | 39.403 | 3.882 | 78.159 | 1.00 | 60.00 |
| ATOM | 1798 | NZ | LYS | 185 | 40.861 | 3.722 | 78.351 | 1.00 | 60.00 |
| ATOM | 1802 | C | LYS | 185 | 34.883 | 3.614 | 77.587 | 1.00 | 60.00 |
| ATOM | 1803 | O | LYS | 185 | 33.880 | 4.162 | 77.131 | 1.00 | 60.00 |
| ATOM | 1804 | N | LEU | 186 | 35.533 | 4.091 | 78.659 | 1.00 | 60.00 |
| ATOM | 1806 | CA | LEU | 186 | 34.995 | 5.238 | 79.314 | 1.00 | 60.00 |
| ATOM | 1807 | CB | LEU | 186 | 35.506 | 5.439 | 80.750 | 1.00 | 60.00 |
| ATOM | 1808 | CG | LEU | 186 | 35.069 | 4.350 | 81.745 | 1.00 | 60.00 |
| ATOM | 1809 | CD1 | LEU | 186 | 35.653 | 2.978 | 81.374 | 1.00 | 60.00 |
| ATOM | 1810 | CD2 | LEU | 186 | 35.392 | 4.768 | 83.189 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1811 | C | LEU | 186 | 35.332 | 6.483 | 78.571 | 1.00 | 60.00 |
| ATOM | 1812 | O | LEU | 186 | 36.484 | 6.913 | 78.546 | 1.00 | 60.00 |
| ATOM | 1813 | N | THR | 187 | 34.321 | 7.095 | 77.925 | 1.00 | 60.00 |
| ATOM | 1815 | CA | THR | 187 | 34.573 | 8.363 | 77.316 | 1.00 | 60.00 |
| ATOM | 1816 | CB | THR | 187 | 33.595 | 8.756 | 76.246 | 1.00 | 60.00 |
| ATOM | 1817 | OG1 | THR | 187 | 34.062 | 9.910 | 75.563 | 1.00 | 60.00 |
| ATOM | 1819 | CG2 | THR | 187 | 32.231 | 9.048 | 76.894 | 1.00 | 60.00 |
| ATOM | 1820 | C | THR | 187 | 34.396 | 9.281 | 78.474 | 1.00 | 60.00 |
| ATOM | 1821 | O | THR | 187 | 33.991 | 8.833 | 79.544 | 1.00 | 60.00 |
| ATOM | 1822 | N | LYS | 188 | 34.687 | 10.584 | 78.305 | 1.00 | 60.00 |
| ATOM | 1824 | CA | LYS | 188 | 34.575 | 11.445 | 79.444 | 1.00 | 60.00 |
| ATOM | 1825 | CB | LYS | 188 | 34.925 | 12.915 | 79.163 | 1.00 | 60.00 |
| ATOM | 1826 | CG | LYS | 188 | 33.900 | 13.660 | 78.310 | 1.00 | 60.00 |
| ATOM | 1827 | CD | LYS | 188 | 34.040 | 15.179 | 78.415 | 1.00 | 60.00 |
| ATOM | 1828 | CE | LYS | 188 | 33.643 | 15.726 | 79.789 | 1.00 | 60.00 |
| ATOM | 1829 | NZ | LYS | 188 | 33.913 | 17.179 | 79.862 | 1.00 | 60.00 |
| ATOM | 1833 | C | LYS | 188 | 33.160 | 11.416 | 79.909 | 1.00 | 60.00 |
| ATOM | 1834 | O | LYS | 188 | 32.887 | 11.311 | 81.104 | 1.00 | 60.00 |
| ATOM | 1835 | N | ILE | 189 | 32.213 | 11.488 | 78.959 | 1.00 | 60.00 |
| ATOM | 1837 | CA | ILE | 189 | 30.839 | 11.477 | 79.346 | 1.00 | 60.00 |
| ATOM | 1838 | CB | ILE | 189 | 29.899 | 11.547 | 78.180 | 1.00 | 60.00 |
| ATOM | 1839 | CG2 | ILE | 189 | 28.472 | 11.349 | 78.715 | 1.00 | 60.00 |
| ATOM | 1840 | CG1 | ILE | 189 | 30.091 | 12.869 | 77.420 | 1.00 | 60.00 |
| ATOM | 1841 | CD1 | ILE | 189 | 29.811 | 14.102 | 78.279 | 1.00 | 60.00 |
| ATOM | 1842 | C | ILE | 189 | 30.579 | 10.189 | 80.048 | 1.00 | 60.00 |
| ATOM | 1843 | O | ILE | 189 | 30.049 | 10.175 | 81.158 | 1.00 | 60.00 |
| ATOM | 1844 | N | ILE | 190 | 30.968 | 9.063 | 79.422 | 1.00 | 60.00 |
| ATOM | 1846 | CA | ILE | 190 | 30.707 | 7.809 | 80.057 | 1.00 | 60.00 |
| ATOM | 1847 | CB | ILE | 190 | 30.069 | 6.798 | 79.136 | 1.00 | 60.00 |
| ATOM | 1848 | CG2 | ILE | 190 | 30.963 | 6.582 | 77.901 | 1.00 | 60.00 |
| ATOM | 1849 | CG1 | ILE | 190 | 29.724 | 5.515 | 79.908 | 1.00 | 60.00 |
| ATOM | 1850 | CD1 | ILE | 190 | 28.793 | 4.578 | 79.140 | 1.00 | 60.00 |
| ATOM | 1851 | C | ILE | 190 | 31.955 | 7.237 | 80.652 | 1.00 | 60.00 |
| ATOM | 1852 | O | ILE | 190 | 32.644 | 6.419 | 80.050 | 1.00 | 60.00 |
| ATOM | 1853 | N | CYS | 191 | 32.266 | 7.679 | 81.882 | 1.00 | 20.00 |
| ATOM | 1855 | CA | CYS | 191 | 33.355 | 7.192 | 82.682 | 1.00 | 20.00 |
| ATOM | 1856 | CB | CYS | 191 | 34.411 | 8.248 | 83.072 | 1.00 | 20.00 |
| ATOM | 1857 | SG | CYS | 191 | 35.657 | 8.621 | 81.806 | 1.00 | 20.00 |
| ATOM | 1858 | C | CYS | 191 | 32.642 | 6.902 | 83.953 | 1.00 | 20.00 |
| ATOM | 1859 | O | CYS | 191 | 31.452 | 6.592 | 83.949 | 1.00 | 20.00 |
| ATOM | 1860 | N | ALA | 192 | 33.354 | 6.979 | 85.089 | 1.00 | 20.00 |
| ATOM | 1862 | CA | ALA | 192 | 32.632 | 6.815 | 86.308 | 1.00 | 20.00 |
| ATOM | 1863 | CB | ALA | 192 | 33.504 | 6.907 | 87.572 | 1.00 | 20.00 |
| ATOM | 1864 | C | ALA | 192 | 31.709 | 7.988 | 86.298 | 1.00 | 20.00 |
| ATOM | 1865 | O | ALA | 192 | 31.983 | 8.996 | 85.650 | 1.00 | 20.00 |
| ATOM | 1866 | N | GLN | 193 | 30.575 | 7.883 | 87.007 | 1.00 | 20.00 |
| ATOM | 1868 | CA | GLN | 193 | 29.623 | 8.951 | 86.991 | 1.00 | 20.00 |
| ATOM | 1869 | CB | GLN | 193 | 28.408 | 8.660 | 87.885 | 1.00 | 20.00 |
| ATOM | 1870 | CG | GLN | 193 | 27.614 | 7.421 | 87.466 | 1.00 | 20.00 |
| ATOM | 1871 | CD | GLN | 193 | 26.463 | 7.264 | 88.448 | 1.00 | 20.00 |
| ATOM | 1872 | OE1 | GLN | 193 | 26.124 | 8.194 | 89.178 | 1.00 | 20.00 |
| ATOM | 1873 | NE2 | GLN | 193 | 25.849 | 6.051 | 88.477 | 1.00 | 20.00 |
| ATOM | 1876 | C | GLN | 193 | 30.284 | 10.164 | 87.555 | 1.00 | 20.00 |
| ATOM | 1877 | O | GLN | 193 | 30.100 | 11.276 | 87.061 | 1.00 | 20.00 |
| ATOM | 1878 | N | GLN | 194 | 31.080 | 9.962 | 88.619 | 1.00 | 20.00 |
| ATOM | 1880 | CA | GLN | 194 | 31.727 | 11.025 | 89.328 | 1.00 | 20.00 |
| ATOM | 1881 | CB | GLN | 194 | 32.421 | 10.520 | 90.602 | 1.00 | 20.00 |
| ATOM | 1882 | CG | GLN | 194 | 31.452 | 9.916 | 91.618 | 1.00 | 20.00 |
| ATOM | 1883 | CD | GLN | 194 | 32.266 | 9.456 | 92.816 | 1.00 | 20.00 |
| ATOM | 1884 | OE1 | GLN | 194 | 31.735 | 8.876 | 93.761 | 1.00 | 20.00 |
| ATOM | 1885 | NE2 | GLN | 194 | 33.600 | 9.717 | 92.775 | 1.00 | 20.00 |
| ATOM | 1888 | C | GLN | 194 | 32.762 | 11.748 | 88.527 | 1.00 | 20.00 |
| ATOM | 1889 | O | GLN | 194 | 32.822 | 12.976 | 88.557 | 1.00 | 20.00 |
| ATOM | 1890 | N | CYS | 195 | 33.601 | 11.012 | 87.775 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1892 | CA | CYS | 195 | 34.677 | 11.669 | 87.090 | 1.00 | 20.00 |
| ATOM | 1893 | CB | CYS | 195 | 35.560 | 10.744 | 86.234 | 1.00 | 20.00 |
| ATOM | 1894 | SG | CYS | 195 | 36.498 | 9.530 | 87.203 | 1.00 | 20.00 |
| ATOM | 1895 | C | CYS | 195 | 34.166 | 12.729 | 86.178 | 1.00 | 20.00 |
| ATOM | 1896 | O | CYS | 195 | 33.102 | 12.601 | 85.575 | 1.00 | 20.00 |
| ATOM | 1897 | N | SER | 196 | 34.923 | 13.837 | 86.088 | 1.00 | 20.00 |
| ATOM | 1899 | CA | SER | 196 | 34.550 | 14.887 | 85.197 | 1.00 | 20.00 |
| ATOM | 1900 | CB | SER | 196 | 34.101 | 16.172 | 85.910 | 1.00 | 20.00 |
| ATOM | 1901 | OG | SER | 196 | 32.911 | 15.924 | 86.644 | 1.00 | 20.00 |
| ATOM | 1903 | C | SER | 196 | 35.763 | 15.221 | 84.395 | 1.00 | 20.00 |
| ATOM | 1904 | O | SER | 196 | 36.859 | 15.369 | 84.932 | 1.00 | 20.00 |
| ATOM | 1905 | N | GLY | 197 | 35.597 | 15.299 | 83.064 | 1.00 | 20.00 |
| ATOM | 1907 | CA | GLY | 197 | 36.671 | 15.699 | 82.207 | 1.00 | 20.00 |
| ATOM | 1908 | C | GLY | 197 | 37.113 | 14.530 | 81.389 | 1.00 | 20.00 |
| ATOM | 1909 | O | GLY | 197 | 36.915 | 14.511 | 80.176 | 1.00 | 20.00 |
| ATOM | 1910 | N | ARG | 198 | 37.712 | 13.515 | 82.048 | 1.00 | 20.00 |
| ATOM | 1912 | CA | ARG | 198 | 38.178 | 12.340 | 81.363 | 1.00 | 20.00 |
| ATOM | 1913 | CB | ARG | 198 | 39.450 | 12.556 | 80.522 | 1.00 | 20.00 |
| ATOM | 1914 | CG | ARG | 198 | 39.207 | 13.349 | 79.238 | 1.00 | 20.00 |
| ATOM | 1915 | CD | ARG | 198 | 38.159 | 12.693 | 78.335 | 1.00 | 20.00 |
| ATOM | 1916 | NE | ARG | 198 | 37.917 | 13.606 | 77.184 | 1.00 | 20.00 |
| ATOM | 1918 | CZ | ARG | 198 | 36.929 | 13.329 | 76.284 | 1.00 | 20.00 |
| ATOM | 1919 | NH1 | ARG | 198 | 36.724 | 14.156 | 75.219 | 1.00 | 20.00 |
| ATOM | 1922 | NH2 | ARG | 198 | 36.145 | 12.222 | 76.452 | 1.00 | 20.00 |
| ATOM | 1925 | C | ARG | 198 | 38.529 | 11.321 | 82.396 | 1.00 | 20.00 |
| ATOM | 1926 | O | ARG | 198 | 38.423 | 11.580 | 83.594 | 1.00 | 20.00 |
| ATOM | 1927 | N | CYS | 199 | 38.930 | 10.109 | 81.955 | 1.00 | 20.00 |
| ATOM | 1929 | CA | CYS | 199 | 39.312 | 9.139 | 82.937 | 1.00 | 20.00 |
| ATOM | 1930 | CB | CYS | 199 | 38.123 | 8.371 | 83.541 | 1.00 | 20.00 |
| ATOM | 1931 | SG | CYS | 199 | 37.204 | 7.408 | 82.306 | 1.00 | 20.00 |
| ATOM | 1932 | C | CYS | 199 | 40.245 | 8.116 | 82.374 | 1.00 | 20.00 |
| ATOM | 1933 | O | CYS | 199 | 40.231 | 7.815 | 81.181 | 1.00 | 20.00 |
| ATOM | 1934 | N | ARG | 200 | 41.117 | 7.581 | 83.252 | 1.00 | 20.00 |
| ATOM | 1936 | CA | ARG | 200 | 42.032 | 6.538 | 82.900 | 1.00 | 20.00 |
| ATOM | 1937 | CB | ARG | 200 | 43.077 | 6.284 | 84.002 | 1.00 | 20.00 |
| ATOM | 1938 | CG | ARG | 200 | 44.151 | 5.262 | 83.625 | 1.00 | 20.00 |
| ATOM | 1939 | CD | ARG | 200 | 43.815 | 3.826 | 84.030 | 1.00 | 20.00 |
| ATOM | 1940 | NE | ARG | 200 | 44.952 | 2.965 | 83.598 | 1.00 | 20.00 |
| ATOM | 1942 | CZ | ARG | 200 | 44.960 | 2.419 | 82.346 | 1.00 | 20.00 |
| ATOM | 1943 | NH1 | ARG | 200 | 43.921 | 2.651 | 81.491 | 1.00 | 20.00 |
| ATOM | 1946 | NH2 | ARG | 200 | 46.010 | 1.641 | 81.951 | 1.00 | 20.00 |
| ATOM | 1949 | C | ARG | 200 | 41.239 | 5.282 | 82.719 | 1.00 | 20.00 |
| ATOM | 1950 | O | ARG | 200 | 41.464 | 4.523 | 81.778 | 1.00 | 20.00 |
| ATOM | 1951 | N | GLY | 201 | 40.266 | 5.045 | 83.622 | 1.00 | 20.00 |
| ATOM | 1953 | CA | GLY | 201 | 39.478 | 3.849 | 83.551 | 1.00 | 20.00 |
| ATOM | 1954 | C | GLY | 201 | 38.275 | 4.028 | 84.422 | 1.00 | 20.00 |
| ATOM | 1955 | O | GLY | 201 | 37.966 | 5.138 | 84.852 | 1.00 | 20.00 |
| ATOM | 1956 | N | LYS | 202 | 37.561 | 2.918 | 84.701 | 1.00 | 20.00 |
| ATOM | 1958 | CA | LYS | 202 | 36.372 | 2.971 | 85.502 | 1.00 | 20.00 |
| ATOM | 1959 | CB | LYS | 202 | 35.473 | 1.729 | 85.344 | 1.00 | 20.00 |
| ATOM | 1960 | CG | LYS | 202 | 34.536 | 1.759 | 84.136 | 1.00 | 20.00 |
| ATOM | 1961 | CD | LYS | 202 | 33.447 | 2.827 | 84.254 | 1.00 | 20.00 |
| ATOM | 1962 | CE | LYS | 202 | 32.464 | 2.569 | 85.398 | 1.00 | 20.00 |
| ATOM | 1963 | NZ | LYS | 202 | 31.492 | 3.680 | 85.500 | 1.00 | 20.00 |
| ATOM | 1967 | C | LYS | 202 | 36.702 | 3.052 | 86.956 | 1.00 | 20.00 |
| ATOM | 1968 | O | LYS | 202 | 36.693 | 2.042 | 87.657 | 1.00 | 20.00 |
| ATOM | 1969 | N | SER | 203 | 37.015 | 4.264 | 87.450 | 1.00 | 20.00 |
| ATOM | 1971 | CA | SER | 203 | 37.229 | 4.428 | 88.857 | 1.00 | 20.00 |
| ATOM | 1972 | CB | SER | 203 | 38.515 | 3.773 | 89.388 | 1.00 | 20.00 |
| ATOM | 1973 | OG | SER | 203 | 39.656 | 4.451 | 88.885 | 1.00 | 20.00 |
| ATOM | 1975 | C | SER | 203 | 37.339 | 5.895 | 89.101 | 1.00 | 20.00 |
| ATOM | 1976 | O | SER | 203 | 37.694 | 6.662 | 88.207 | 1.00 | 20.00 |
| ATOM | 1977 | N | PRO | 204 | 37.009 | 6.306 | 90.290 | 1.00 | 20.00 |
| ATOM | 1978 | CD | PRO | 204 | 35.914 | 5.677 | 91.012 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1979 | CA | PRO | 204 | 37.136 | 7.697 | 90.613 | 1.00 | 20.00 |
| ATOM | 1980 | CB | PRO | 204 | 36.361 | 7.894 | 91.912 | 1.00 | 20.00 |
| ATOM | 1981 | CG | PRO | 204 | 35.277 | 6.800 | 91.847 | 1.00 | 20.00 |
| ATOM | 1982 | C | PRO | 204 | 38.584 | 8.051 | 90.685 | 1.00 | 20.00 |
| ATOM | 1983 | O | PRO | 204 | 38.925 | 9.227 | 90.563 | 1.00 | 20.00 |
| ATOM | 1984 | N | SER | 205 | 39.445 | 7.045 | 90.920 | 1.00 | 20.00 |
| ATOM | 1986 | CA | SER | 205 | 40.861 | 7.250 | 90.973 | 1.00 | 20.00 |
| ATOM | 1987 | CB | SER | 205 | 41.623 | 5.985 | 91.400 | 1.00 | 20.00 |
| ATOM | 1988 | OG | SER | 205 | 41.259 | 5.621 | 92.723 | 1.00 | 20.00 |
| ATOM | 1990 | C | SER | 205 | 41.298 | 7.589 | 89.587 | 1.00 | 20.00 |
| ATOM | 1991 | O | SER | 205 | 42.189 | 8.412 | 89.379 | 1.00 | 20.00 |
| ATOM | 1992 | N | ASP | 206 | 40.643 | 6.948 | 88.604 | 1.00 | 20.00 |
| ATOM | 1994 | CA | ASP | 206 | 40.948 | 7.079 | 87.212 | 1.00 | 20.00 |
| ATOM | 1995 | CB | ASP | 206 | 40.180 | 6.094 | 86.316 | 1.00 | 20.00 |
| ATOM | 1996 | CG | ASP | 206 | 40.887 | 4.749 | 86.409 | 1.00 | 20.00 |
| ATOM | 1997 | OD1 | ASP | 206 | 40.184 | 3.704 | 86.368 | 1.00 | 20.00 |
| ATOM | 1998 | OD2 | ASP | 206 | 42.142 | 4.751 | 86.518 | 1.00 | 20.00 |
| ATOM | 1999 | C | ASP | 206 | 40.703 | 8.452 | 86.687 | 1.00 | 20.00 |
| ATOM | 2000 | O | ASP | 206 | 41.286 | 8.800 | 85.661 | 1.00 | 20.00 |
| ATOM | 2001 | N | CYS | 207 | 39.811 | 9.229 | 87.348 | 1.00 | 20.00 |
| ATOM | 2003 | CA | CYS | 207 | 39.456 | 10.559 | 86.921 | 1.00 | 20.00 |
| ATOM | 2004 | CB | CYS | 207 | 38.758 | 11.404 | 88.000 | 1.00 | 20.00 |
| ATOM | 2005 | SG | CYS | 207 | 37.287 | 10.620 | 88.721 | 1.00 | 20.00 |
| ATOM | 2006 | C | CYS | 207 | 40.702 | 11.297 | 86.535 | 1.00 | 20.00 |
| ATOM | 2007 | O | CYS | 207 | 41.765 | 11.068 | 87.110 | 1.00 | 20.00 |
| ATOM | 2008 | N | CYS | 208 | 40.612 | 12.192 | 85.530 | 1.00 | 20.00 |
| ATOM | 2010 | CA | CYS | 208 | 41.814 | 12.830 | 85.073 | 1.00 | 20.00 |
| ATOM | 2011 | CB | CYS | 208 | 42.132 | 12.584 | 83.584 | 1.00 | 20.00 |
| ATOM | 2012 | SG | CYS | 208 | 43.890 | 12.887 | 83.236 | 1.00 | 20.00 |
| ATOM | 2013 | C | CYS | 208 | 41.703 | 14.311 | 85.255 | 1.00 | 20.00 |
| ATOM | 2014 | O | CYS | 208 | 40.680 | 14.824 | 85.707 | 1.00 | 20.00 |
| ATOM | 2015 | N | HIS | 209 | 42.788 | 15.037 | 84.915 | 1.00 | 20.00 |
| ATOM | 2017 | CA | HIS | 209 | 42.827 | 16.460 | 85.083 | 1.00 | 20.00 |
| ATOM | 2018 | CB | HIS | 209 | 44.187 | 17.074 | 84.698 | 1.00 | 20.00 |
| ATOM | 2019 | CG | HIS | 209 | 44.306 | 18.531 | 85.033 | 1.00 | 20.00 |
| ATOM | 2020 | CD2 | HIS | 209 | 44.765 | 19.137 | 86.163 | 1.00 | 20.00 |
| ATOM | 2021 | ND1 | HIS | 209 | 43.946 | 19.550 | 84.181 | 1.00 | 20.00 |
| ATOM | 2023 | CE1 | HIS | 209 | 44.203 | 20.713 | 84.830 | 1.00 | 20.00 |
| ATOM | 2024 | NE2 | HIS | 209 | 44.701 | 20.513 | 86.037 | 1.00 | 20.00 |
| ATOM | 2026 | C | HIS | 209 | 41.760 | 17.080 | 84.239 | 1.00 | 20.00 |
| ATOM | 2027 | O | HIS | 209 | 41.311 | 16.503 | 83.251 | 1.00 | 20.00 |
| ATOM | 2028 | N | ASN | 210 | 41.317 | 18.289 | 84.632 | 1.00 | 20.00 |
| ATOM | 2030 | CA | ASN | 210 | 40.255 | 18.971 | 83.952 | 1.00 | 20.00 |
| ATOM | 2031 | CB | ASN | 210 | 39.810 | 20.259 | 84.670 | 1.00 | 20.00 |
| ATOM | 2032 | CG | ASN | 210 | 40.987 | 21.221 | 84.745 | 1.00 | 20.00 |
| ATOM | 2033 | OD1 | ASN | 210 | 41.375 | 21.838 | 83.754 | 1.00 | 20.00 |
| ATOM | 2034 | ND2 | ASN | 210 | 41.562 | 21.368 | 85.969 | 1.00 | 20.00 |
| ATOM | 2037 | C | ASN | 210 | 40.644 | 19.322 | 82.547 | 1.00 | 20.00 |
| ATOM | 2038 | O | ASN | 210 | 39.809 | 19.293 | 81.644 | 1.00 | 20.00 |
| ATOM | 2039 | N | GLN | 211 | 41.920 | 19.698 | 82.340 | 1.00 | 20.00 |
| ATOM | 2041 | CA | GLN | 211 | 42.433 | 20.094 | 81.056 | 1.00 | 20.00 |
| ATOM | 2042 | CB | GLN | 211 | 43.817 | 20.754 | 81.156 | 1.00 | 20.00 |
| ATOM | 2043 | CG | GLN | 211 | 43.804 | 22.051 | 81.966 | 1.00 | 20.00 |
| ATOM | 2044 | CD | GLN | 211 | 42.967 | 23.077 | 81.212 | 1.00 | 20.00 |
| ATOM | 2045 | OE1 | GLN | 211 | 42.714 | 22.936 | 80.016 | 1.00 | 20.00 |
| ATOM | 2046 | NE2 | GLN | 211 | 42.528 | 24.144 | 81.931 | 1.00 | 20.00 |
| ATOM | 2049 | C | GLN | 211 | 42.545 | 18.956 | 80.093 | 1.00 | 20.00 |
| ATOM | 2050 | O | GLN | 211 | 42.326 | 19.106 | 78.892 | 1.00 | 20.00 |
| ATOM | 2051 | N | CYS | 212 | 42.911 | 17.779 | 80.608 | 1.00 | 20.00 |
| ATOM | 2053 | CA | CYS | 212 | 43.108 | 16.604 | 79.822 | 1.00 | 20.00 |
| ATOM | 2054 | CB | CYS | 212 | 43.214 | 15.421 | 80.762 | 1.00 | 20.00 |
| ATOM | 2055 | SG | CYS | 212 | 44.657 | 15.757 | 81.777 | 1.00 | 20.00 |
| ATOM | 2056 | C | CYS | 212 | 41.941 | 16.393 | 78.929 | 1.00 | 20.00 |
| ATOM | 2057 | O | CYS | 212 | 40.802 | 16.652 | 79.309 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2058 | N | ALA | 213 | 42.212 | 15.952 | 77.688 | 1.00 | 20.00 |
| ATOM | 2060 | CA | ALA | 213 | 41.143 | 15.660 | 76.792 | 1.00 | 20.00 |
| ATOM | 2061 | CB | ALA | 213 | 41.084 | 16.582 | 75.562 | 1.00 | 20.00 |
| ATOM | 2062 | C | ALA | 213 | 41.425 | 14.273 | 76.320 | 1.00 | 20.00 |
| ATOM | 2063 | O | ALA | 213 | 42.577 | 13.844 | 76.300 | 1.00 | 20.00 |
| ATOM | 2064 | N | ALA | 214 | 40.368 | 13.525 | 75.957 | 1.00 | 20.00 |
| ATOM | 2066 | CA | ALA | 214 | 40.528 | 12.175 | 75.504 | 1.00 | 20.00 |
| ATOM | 2067 | CB | ALA | 214 | 41.699 | 11.962 | 74.525 | 1.00 | 20.00 |
| ATOM | 2068 | C | ALA | 214 | 40.711 | 11.263 | 76.677 | 1.00 | 20.00 |
| ATOM | 2069 | O | ALA | 214 | 39.751 | 10.646 | 77.138 | 1.00 | 20.00 |
| ATOM | 2070 | N | GLY | 215 | 41.955 | 11.149 | 77.192 | 1.00 | 20.00 |
| ATOM | 2072 | CA | GLY | 215 | 42.196 | 10.264 | 78.303 | 1.00 | 20.00 |
| ATOM | 2073 | C | GLY | 215 | 43.502 | 10.625 | 78.944 | 1.00 | 20.00 |
| ATOM | 2074 | O | GLY | 215 | 43.975 | 11.754 | 78.818 | 1.00 | 20.00 |
| ATOM | 2075 | N | CYS | 216 | 44.101 | 9.684 | 79.707 | 1.00 | 20.00 |
| ATOM | 2077 | CA | CYS | 216 | 45.376 | 9.987 | 80.283 | 1.00 | 20.00 |
| ATOM | 2078 | CB | CYS | 216 | 45.343 | 11.252 | 81.161 | 1.00 | 20.00 |
| ATOM | 2079 | SG | CYS | 216 | 44.623 | 11.038 | 82.816 | 1.00 | 20.00 |
| ATOM | 2080 | C | CYS | 216 | 45.875 | 8.808 | 81.064 | 1.00 | 20.00 |
| ATOM | 2081 | O | CYS | 216 | 45.119 | 7.884 | 81.362 | 1.00 | 20.00 |
| ATOM | 2082 | N | THR | 217 | 47.189 | 8.779 | 81.372 | 1.00 | 20.00 |
| ATOM | 2084 | CA | THR | 217 | 47.714 | 7.670 | 82.119 | 1.00 | 20.00 |
| ATOM | 2085 | CB | THR | 217 | 49.218 | 7.605 | 82.163 | 1.00 | 20.00 |
| ATOM | 2086 | OG1 | THR | 217 | 49.627 | 6.333 | 82.641 | 1.00 | 20.00 |
| ATOM | 2088 | CG2 | THR | 217 | 49.764 | 8.698 | 83.093 | 1.00 | 20.00 |
| ATOM | 2089 | C | THR | 217 | 47.201 | 7.681 | 83.529 | 1.00 | 20.00 |
| ATOM | 2090 | O | THR | 217 | 46.827 | 6.639 | 84.065 | 1.00 | 20.00 |
| ATOM | 2091 | N | GLY | 218 | 47.162 | 8.869 | 84.167 | 1.00 | 20.00 |
| ATOM | 2093 | CA | GLY | 218 | 46.700 | 8.971 | 85.525 | 1.00 | 20.00 |
| ATOM | 2094 | C | GLY | 218 | 46.499 | 10.427 | 85.785 | 1.00 | 20.00 |
| ATOM | 2095 | O | GLY | 218 | 47.164 | 11.256 | 85.168 | 1.00 | 20.00 |
| ATOM | 2096 | N | PRO | 219 | 45.620 | 10.765 | 86.692 | 1.00 | 40.00 |
| ATOM | 2097 | CD | PRO | 219 | 45.358 | 9.917 | 87.844 | 1.00 | 40.00 |
| ATOM | 2098 | CA | PRO | 219 | 45.286 | 12.142 | 86.948 | 1.00 | 40.00 |
| ATOM | 2099 | CB | PRO | 219 | 44.421 | 12.125 | 88.206 | 1.00 | 40.00 |
| ATOM | 2100 | CG | PRO | 219 | 44.931 | 10.884 | 88.961 | 1.00 | 40.00 |
| ATOM | 2101 | C | PRO | 219 | 46.484 | 13.028 | 87.106 | 1.00 | 40.00 |
| ATOM | 2102 | O | PRO | 219 | 47.146 | 12.971 | 88.140 | 1.00 | 40.00 |
| ATOM | 2103 | N | ARG | 220 | 46.763 | 13.856 | 86.079 | 1.00 | 40.00 |
| ATOM | 2105 | CA | ARG | 220 | 47.847 | 14.791 | 86.092 | 1.00 | 40.00 |
| ATOM | 2106 | CB | ARG | 220 | 49.241 | 14.143 | 86.156 | 1.00 | 40.00 |
| ATOM | 2107 | CG | ARG | 220 | 50.377 | 15.168 | 86.169 | 1.00 | 40.00 |
| ATOM | 2108 | CD | ARG | 220 | 51.759 | 14.562 | 86.416 | 1.00 | 40.00 |
| ATOM | 2109 | NE | ARG | 220 | 51.806 | 14.132 | 87.842 | 1.00 | 40.00 |
| ATOM | 2111 | CZ | ARG | 220 | 51.345 | 12.899 | 88.204 | 1.00 | 40.00 |
| ATOM | 2112 | NH1 | ARG | 220 | 51.379 | 12.520 | 89.515 | 1.00 | 40.00 |
| ATOM | 2115 | NH2 | ARG | 220 | 50.852 | 12.044 | 87.262 | 1.00 | 40.00 |
| ATOM | 2118 | C | ARG | 220 | 47.752 | 15.546 | 84.804 | 1.00 | 40.00 |
| ATOM | 2119 | O | ARG | 220 | 47.161 | 15.067 | 83.839 | 1.00 | 40.00 |
| ATOM | 2120 | N | GLU | 221 | 48.316 | 16.765 | 84.767 | 1.00 | 20.00 |
| ATOM | 2122 | CA | GLU | 221 | 48.290 | 17.606 | 83.602 | 1.00 | 20.00 |
| ATOM | 2123 | CB | GLU | 221 | 48.797 | 19.024 | 83.910 | 1.00 | 20.00 |
| ATOM | 2124 | CG | GLU | 221 | 47.920 | 19.795 | 84.898 | 1.00 | 20.00 |
| ATOM | 2125 | CD | GLU | 221 | 48.628 | 21.101 | 85.230 | 1.00 | 20.00 |
| ATOM | 2126 | OE1 | GLU | 221 | 48.993 | 21.839 | 84.276 | 1.00 | 20.00 |
| ATOM | 2127 | OE2 | GLU | 221 | 48.817 | 21.375 | 86.446 | 1.00 | 20.00 |
| ATOM | 2128 | C | GLU | 221 | 49.156 | 17.082 | 82.491 | 1.00 | 20.00 |
| ATOM | 2129 | O | GLU | 221 | 48.814 | 17.193 | 81.316 | 1.00 | 20.00 |
| ATOM | 2130 | N | SER | 222 | 50.334 | 16.539 | 82.848 | 1.00 | 20.00 |
| ATOM | 2132 | CA | SER | 222 | 51.324 | 16.099 | 81.902 | 1.00 | 20.00 |
| ATOM | 2133 | CB | SER | 222 | 52.691 | 15.855 | 82.565 | 1.00 | 20.00 |
| ATOM | 2134 | OG | SER | 222 | 52.603 | 14.778 | 83.487 | 1.00 | 20.00 |
| ATOM | 2136 | C | SER | 222 | 50.999 | 14.860 | 81.120 | 1.00 | 20.00 |
| ATOM | 2137 | O | SER | 222 | 51.361 | 14.741 | 79.952 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2138 | N | ASP | 223 | 50.342 | 13.881 | 81.759 | 1.00 | 20.00 |
| ATOM | 2140 | CA | ASP | 223 | 50.110 | 12.593 | 81.165 | 1.00 | 20.00 |
| ATOM | 2141 | CB | ASP | 223 | 49.830 | 11.500 | 82.195 | 1.00 | 20.00 |
| ATOM | 2142 | CG | ASP | 223 | 48.518 | 11.829 | 82.857 | 1.00 | 20.00 |
| ATOM | 2143 | OD1 | ASP | 223 | 47.585 | 11.000 | 82.697 | 1.00 | 20.00 |
| ATOM | 2144 | OD2 | ASP | 223 | 48.422 | 12.888 | 83.529 | 1.00 | 20.00 |
| ATOM | 2145 | C | ASP | 223 | 49.059 | 12.514 | 80.099 | 1.00 | 20.00 |
| ATOM | 2146 | O | ASP | 223 | 48.972 | 11.524 | 79.377 | 1.00 | 20.00 |
| ATOM | 2147 | N | CYS | 224 | 48.181 | 13.518 | 80.001 | 1.00 | 20.00 |
| ATOM | 2149 | CA | CYS | 224 | 47.069 | 13.416 | 79.106 | 1.00 | 20.00 |
| ATOM | 2150 | CB | CYS | 224 | 46.143 | 14.588 | 79.372 | 1.00 | 20.00 |
| ATOM | 2151 | SG | CYS | 224 | 45.836 | 14.280 | 81.137 | 1.00 | 20.00 |
| ATOM | 2152 | C | CYS | 224 | 47.403 | 13.115 | 77.677 | 1.00 | 20.00 |
| ATOM | 2153 | O | CYS | 224 | 48.507 | 13.379 | 77.209 | 1.00 | 20.00 |
| ATOM | 2154 | N | LEU | 225 | 46.474 | 12.399 | 77.001 | 1.00 | 20.00 |
| ATOM | 2156 | CA | LEU | 225 | 46.601 | 12.001 | 75.627 | 1.00 | 20.00 |
| ATOM | 2157 | CB | LEU | 225 | 45.630 | 10.880 | 75.219 | 1.00 | 20.00 |
| ATOM | 2158 | CG | LEU | 225 | 45.984 | 9.523 | 75.857 | 1.00 | 20.00 |
| ATOM | 2159 | CD1 | LEU | 225 | 45.831 | 9.559 | 77.387 | 1.00 | 20.00 |
| ATOM | 2160 | CD2 | LEU | 225 | 45.207 | 8.373 | 75.198 | 1.00 | 20.00 |
| ATOM | 2161 | C | LEU | 225 | 46.402 | 13.160 | 74.708 | 1.00 | 20.00 |
| ATOM | 2162 | O | LEU | 225 | 46.995 | 13.214 | 73.631 | 1.00 | 20.00 |
| ATOM | 2163 | N | VAL | 226 | 45.504 | 14.090 | 75.082 | 1.00 | 20.00 |
| ATOM | 2165 | CA | VAL | 226 | 45.314 | 15.266 | 74.290 | 1.00 | 20.00 |
| ATOM | 2166 | CB | VAL | 226 | 44.276 | 15.130 | 73.206 | 1.00 | 20.00 |
| ATOM | 2167 | CG1 | VAL | 226 | 42.883 | 14.999 | 73.839 | 1.00 | 20.00 |
| ATOM | 2168 | CG2 | VAL | 226 | 44.408 | 16.330 | 72.253 | 1.00 | 20.00 |
| ATOM | 2169 | C | VAL | 226 | 44.898 | 16.356 | 75.224 | 1.00 | 20.00 |
| ATOM | 2170 | O | VAL | 226 | 44.618 | 16.100 | 76.395 | 1.00 | 20.00 |
| ATOM | 2171 | N | CYS | 227 | 44.864 | 17.613 | 74.730 | 1.00 | 20.00 |
| ATOM | 2173 | CA | CYS | 227 | 44.543 | 18.697 | 75.608 | 1.00 | 20.00 |
| ATOM | 2174 | CB | CYS | 227 | 45.567 | 19.841 | 75.570 | 1.00 | 20.00 |
| ATOM | 2175 | SG | CYS | 227 | 47.232 | 19.319 | 76.080 | 1.00 | 20.00 |
| ATOM | 2176 | C | CYS | 227 | 43.223 | 19.274 | 75.223 | 1.00 | 20.00 |
| ATOM | 2177 | O | CYS | 227 | 42.833 | 19.255 | 74.056 | 1.00 | 20.00 |
| ATOM | 2178 | N | ARG | 228 | 42.474 | 19.758 | 76.233 | 1.00 | 20.00 |
| ATOM | 2180 | CA | ARG | 228 | 41.201 | 20.357 | 75.988 | 1.00 | 20.00 |
| ATOM | 2181 | CB | ARG | 228 | 40.368 | 20.572 | 77.259 | 1.00 | 20.00 |
| ATOM | 2182 | CG | ARG | 228 | 38.907 | 20.875 | 76.928 | 1.00 | 20.00 |
| ATOM | 2183 | CD | ARG | 228 | 37.939 | 20.635 | 78.084 | 1.00 | 20.00 |
| ATOM | 2184 | NE | ARG | 228 | 36.571 | 20.659 | 77.498 | 1.00 | 20.00 |
| ATOM | 2186 | CZ | ARG | 228 | 36.083 | 19.543 | 76.880 | 1.00 | 20.00 |
| ATOM | 2187 | NH1 | ARG | 228 | 36.848 | 18.415 | 76.804 | 1.00 | 20.00 |
| ATOM | 2190 | NH2 | ARG | 228 | 34.836 | 19.558 | 76.326 | 1.00 | 20.00 |
| ATOM | 2193 | C | ARG | 228 | 41.409 | 21.673 | 75.318 | 1.00 | 20.00 |
| ATOM | 2194 | O | ARG | 228 | 40.688 | 22.039 | 74.391 | 1.00 | 20.00 |
| ATOM | 2195 | N | LYS | 229 | 42.443 | 22.406 | 75.766 | 1.00 | 20.00 |
| ATOM | 2197 | CA | LYS | 229 | 42.692 | 23.714 | 75.244 | 1.00 | 20.00 |
| ATOM | 2198 | CB | LYS | 229 | 42.841 | 24.767 | 76.353 | 1.00 | 20.00 |
| ATOM | 2199 | CG | LYS | 229 | 41.624 | 24.772 | 77.280 | 1.00 | 20.00 |
| ATOM | 2200 | CD | LYS | 229 | 40.295 | 24.908 | 76.533 | 1.00 | 20.00 |
| ATOM | 2201 | CE | LYS | 229 | 39.074 | 24.570 | 77.392 | 1.00 | 20.00 |
| ATOM | 2202 | NZ | LYS | 229 | 37.854 | 24.553 | 76.554 | 1.00 | 20.00 |
| ATOM | 2206 | C | LYS | 229 | 43.956 | 23.664 | 74.448 | 1.00 | 20.00 |
| ATOM | 2207 | O | LYS | 229 | 44.019 | 23.016 | 73.403 | 1.00 | 20.00 |
| ATOM | 2208 | N | PHE | 230 | 45.000 | 24.379 | 74.908 | 1.00 | 20.00 |
| ATOM | 2210 | CA | PHE | 230 | 46.218 | 24.397 | 74.149 | 1.00 | 20.00 |
| ATOM | 2211 | CB | PHE | 230 | 46.761 | 25.815 | 73.900 | 1.00 | 20.00 |
| ATOM | 2212 | CG | PHE | 230 | 45.779 | 26.531 | 73.039 | 1.00 | 20.00 |
| ATOM | 2213 | CD1 | PHE | 230 | 44.688 | 27.156 | 73.599 | 1.00 | 20.00 |
| ATOM | 2214 | CD2 | PHE | 230 | 45.955 | 26.592 | 71.677 | 1.00 | 20.00 |
| ATOM | 2215 | CE1 | PHE | 230 | 43.786 | 27.829 | 72.809 | 1.00 | 20.00 |
| ATOM | 2216 | CE2 | PHE | 230 | 45.058 | 27.265 | 70.882 | 1.00 | 20.00 |
| ATOM | 2217 | CZ | PHE | 230 | 43.970 | 27.884 | 71.448 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2218 | C | PHE | 230 | 47.283 | 23.651 | 74.882 | 1.00 | 20.00 |
| ATOM | 2219 | O | PHE | 230 | 47.373 | 23.717 | 76.105 | 1.00 | 20.00 |
| ATOM | 2220 | N | ARG | 231 | 48.130 | 22.916 | 74.135 | 1.00 | 20.00 |
| ATOM | 2222 | CA | ARG | 231 | 49.172 | 22.161 | 74.761 | 1.00 | 20.00 |
| ATOM | 2223 | CB | ARG | 231 | 49.466 | 20.819 | 74.071 | 1.00 | 20.00 |
| ATOM | 2224 | CG | ARG | 231 | 50.426 | 19.926 | 74.861 | 1.00 | 20.00 |
| ATOM | 2225 | CD | ARG | 231 | 51.000 | 18.772 | 74.036 | 1.00 | 20.00 |
| ATOM | 2226 | NE | ARG | 231 | 49.855 | 18.058 | 73.407 | 1.00 | 20.00 |
| ATOM | 2228 | CZ | ARG | 231 | 50.080 | 17.186 | 72.382 | 1.00 | 20.00 |
| ATOM | 2229 | NH1 | ARG | 231 | 51.359 | 16.908 | 71.991 | 1.00 | 20.00 |
| ATOM | 2232 | NH2 | ARG | 231 | 49.025 | 16.602 | 71.746 | 1.00 | 20.00 |
| ATOM | 2235 | C | ARG | 231 | 50.423 | 22.969 | 74.676 | 1.00 | 20.00 |
| ATOM | 2236 | O | ARG | 231 | 50.752 | 23.510 | 73.621 | 1.00 | 20.00 |
| ATOM | 2237 | N | ASP | 232 | 51.144 | 23.103 | 75.804 | 1.00 | 20.00 |
| ATOM | 2239 | CA | ASP | 232 | 52.359 | 23.853 | 75.739 | 1.00 | 20.00 |
| ATOM | 2240 | CB | ASP | 232 | 52.188 | 25.331 | 76.136 | 1.00 | 20.00 |
| ATOM | 2241 | CG | ASP | 232 | 53.432 | 26.092 | 75.694 | 1.00 | 20.00 |
| ATOM | 2242 | OD1 | ASP | 232 | 53.480 | 27.330 | 75.921 | 1.00 | 20.00 |
| ATOM | 2243 | OD2 | ASP | 232 | 54.346 | 25.446 | 75.114 | 1.00 | 20.00 |
| ATOM | 2244 | C | ASP | 232 | 53.358 | 23.243 | 76.667 | 1.00 | 20.00 |
| ATOM | 2245 | O | ASP | 232 | 53.050 | 22.936 | 77.816 | 1.00 | 20.00 |
| ATOM | 2246 | N | GLU | 233 | 54.597 | 23.062 | 76.174 | 1.00 | 20.00 |
| ATOM | 2248 | CA | GLU | 233 | 55.662 | 22.517 | 76.963 | 1.00 | 20.00 |
| ATOM | 2249 | CB | GLU | 233 | 56.221 | 23.517 | 77.989 | 1.00 | 20.00 |
| ATOM | 2250 | CG | GLU | 233 | 56.969 | 24.685 | 77.346 | 1.00 | 20.00 |
| ATOM | 2251 | CD | GLU | 233 | 58.294 | 24.153 | 76.822 | 1.00 | 20.00 |
| ATOM | 2252 | OE1 | GLU | 233 | 59.095 | 23.647 | 77.652 | 1.00 | 20.00 |
| ATOM | 2253 | OE2 | GLU | 233 | 58.524 | 24.243 | 75.586 | 1.00 | 20.00 |
| ATOM | 2254 | C | GLU | 233 | 55.237 | 21.291 | 77.701 | 1.00 | 20.00 |
| ATOM | 2255 | O | GLU | 233 | 55.325 | 21.232 | 78.926 | 1.00 | 20.00 |
| ATOM | 2256 | N | ALA | 234 | 54.756 | 20.278 | 76.961 | 1.00 | 20.00 |
| ATOM | 2258 | CA | ALA | 234 | 54.388 | 19.025 | 77.554 | 1.00 | 20.00 |
| ATOM | 2259 | CB | ALA | 234 | 55.569 | 18.320 | 78.244 | 1.00 | 20.00 |
| ATOM | 2260 | C | ALA | 234 | 53.298 | 19.181 | 78.564 | 1.00 | 20.00 |
| ATOM | 2261 | O | ALA | 234 | 52.972 | 18.229 | 79.270 | 1.00 | 20.00 |
| ATOM | 2262 | N | THR | 235 | 52.681 | 20.374 | 78.663 | 1.00 | 20.00 |
| ATOM | 2264 | CA | THR | 235 | 51.626 | 20.486 | 79.626 | 1.00 | 20.00 |
| ATOM | 2265 | CB | THR | 235 | 51.897 | 21.482 | 80.717 | 1.00 | 20.00 |
| ATOM | 2266 | OG1 | THR | 235 | 52.016 | 22.789 | 80.175 | 1.00 | 20.00 |
| ATOM | 2268 | CG2 | THR | 235 | 53.198 | 21.086 | 81.434 | 1.00 | 20.00 |
| ATOM | 2269 | C | THR | 235 | 50.387 | 20.928 | 78.924 | 1.00 | 20.00 |
| ATOM | 2270 | O | THR | 235 | 50.447 | 21.651 | 77.930 | 1.00 | 20.00 |
| ATOM | 2271 | N | CYS | 236 | 49.216 | 20.483 | 79.421 | 1.00 | 20.00 |
| ATOM | 2273 | CA | CYS | 236 | 47.989 | 20.894 | 78.810 | 1.00 | 20.00 |
| ATOM | 2274 | CB | CYS | 236 | 46.819 | 19.910 | 78.989 | 1.00 | 20.00 |
| ATOM | 2275 | SG | CYS | 236 | 46.939 | 18.467 | 77.899 | 1.00 | 20.00 |
| ATOM | 2276 | C | CYS | 236 | 47.599 | 22.168 | 79.473 | 1.00 | 20.00 |
| ATOM | 2277 | O | CYS | 236 | 47.313 | 22.189 | 80.669 | 1.00 | 20.00 |
| ATOM | 2278 | N | LYS | 237 | 47.579 | 23.269 | 78.694 | 1.00 | 20.00 |
| ATOM | 2280 | CA | LYS | 237 | 47.273 | 24.556 | 79.241 | 1.00 | 20.00 |
| ATOM | 2281 | CB | LYS | 237 | 48.296 | 25.640 | 78.862 | 1.00 | 20.00 |
| ATOM | 2282 | CG | LYS | 237 | 49.668 | 25.442 | 79.509 | 1.00 | 20.00 |
| ATOM | 2283 | CD | LYS | 237 | 50.763 | 26.323 | 78.905 | 1.00 | 20.00 |
| ATOM | 2284 | CE | LYS | 237 | 52.133 | 26.124 | 79.556 | 1.00 | 20.00 |
| ATOM | 2285 | NZ | LYS | 237 | 53.141 | 26.973 | 78.882 | 1.00 | 20.00 |
| ATOM | 2289 | C | LYS | 237 | 45.937 | 25.018 | 78.754 | 1.00 | 20.00 |
| ATOM | 2290 | O | LYS | 237 | 45.538 | 24.748 | 77.623 | 1.00 | 20.00 |
| ATOM | 2291 | N | ASP | 238 | 45.193 | 25.697 | 79.650 | 1.00 | 20.00 |
| ATOM | 2293 | CA | ASP | 238 | 43.904 | 26.249 | 79.350 | 1.00 | 20.00 |
| ATOM | 2294 | CB | ASP | 238 | 43.207 | 26.805 | 80.606 | 1.00 | 20.00 |
| ATOM | 2295 | CG | ASP | 238 | 41.761 | 27.127 | 80.258 | 1.00 | 20.00 |
| ATOM | 2296 | OD1 | ASP | 238 | 41.399 | 27.014 | 79.057 | 1.00 | 20.00 |
| ATOM | 2297 | OD2 | ASP | 238 | 40.999 | 27.492 | 81.194 | 1.00 | 20.00 |
| ATOM | 2298 | C | ASP | 238 | 44.080 | 27.378 | 78.383 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2299 | O | ASP | 238 | 43.294 | 27.553 | 77.452 | 1.00 | 20.00 |
| ATOM | 2300 | N | THR | 239 | 45.124 | 28.195 | 78.604 | 1.00 | 20.00 |
| ATOM | 2302 | CA | THR | 239 | 45.395 | 29.288 | 77.721 | 1.00 | 20.00 |
| ATOM | 2303 | CB | THR | 239 | 44.901 | 30.613 | 78.222 | 1.00 | 20.00 |
| ATOM | 2304 | OG1 | THR | 239 | 45.004 | 31.594 | 77.201 | 1.00 | 20.00 |
| ATOM | 2306 | CG2 | THR | 239 | 45.744 | 31.022 | 79.442 | 1.00 | 20.00 |
| ATOM | 2307 | C | THR | 239 | 46.879 | 29.365 | 77.641 | 1.00 | 20.00 |
| ATOM | 2308 | O | THR | 239 | 47.581 | 28.773 | 78.459 | 1.00 | 20.00 |
| ATOM | 2309 | N | CYS | 240 | 47.410 | 30.087 | 76.640 | 1.00 | 20.00 |
| ATOM | 2311 | CA | CYS | 240 | 48.835 | 30.120 | 76.543 | 1.00 | 20.00 |
| ATOM | 2312 | CB | CYS | 240 | 49.340 | 30.107 | 75.100 | 1.00 | 20.00 |
| ATOM | 2313 | SG | CYS | 240 | 49.026 | 28.455 | 74.421 | 1.00 | 20.00 |
| ATOM | 2314 | C | CYS | 240 | 49.397 | 31.268 | 77.303 | 1.00 | 20.00 |
| ATOM | 2315 | O | CYS | 240 | 48.974 | 32.417 | 77.198 | 1.00 | 20.00 |
| ATOM | 2316 | N | PRO | 241 | 50.343 | 30.894 | 78.119 | 1.00 | 40.00 |
| ATOM | 2317 | CD | PRO | 241 | 50.319 | 29.560 | 78.691 | 1.00 | 40.00 |
| ATOM | 2318 | CA | PRO | 241 | 51.014 | 31.831 | 78.973 | 1.00 | 40.00 |
| ATOM | 2319 | CB | PRO | 241 | 51.531 | 31.028 | 80.169 | 1.00 | 40.00 |
| ATOM | 2320 | CG | PRO | 241 | 51.463 | 29.562 | 79.714 | 1.00 | 40.00 |
| ATOM | 2321 | C | PRO | 241 | 52.097 | 32.561 | 78.253 | 1.00 | 40.00 |
| ATOM | 2322 | O | PRO | 241 | 52.520 | 32.130 | 77.181 | 1.00 | 40.00 |
| ATOM | 2323 | N | PRO | 242 | 52.520 | 33.654 | 78.820 | 1.00 | 60.00 |
| ATOM | 2324 | CD | PRO | 242 | 51.564 | 34.527 | 79.485 | 1.00 | 60.00 |
| ATOM | 2325 | CA | PRO | 242 | 53.598 | 34.393 | 78.227 | 1.00 | 60.00 |
| ATOM | 2326 | CB | PRO | 242 | 53.501 | 35.808 | 78.793 | 1.00 | 60.00 |
| ATOM | 2327 | CG | PRO | 242 | 52.014 | 35.959 | 79.154 | 1.00 | 60.00 |
| ATOM | 2328 | C | PRO | 242 | 54.875 | 33.709 | 78.587 | 1.00 | 60.00 |
| ATOM | 2329 | O | PRO | 242 | 54.870 | 32.896 | 79.510 | 1.00 | 60.00 |
| ATOM | 2330 | N | LEU | 243 | 55.978 | 34.015 | 77.877 | 1.00 | 60.00 |
| ATOM | 2332 | CA | LEU | 243 | 57.227 | 33.396 | 78.202 | 1.00 | 60.00 |
| ATOM | 2333 | CB | LEU | 243 | 58.383 | 33.812 | 77.277 | 1.00 | 60.00 |
| ATOM | 2334 | CG | LEU | 243 | 59.726 | 33.148 | 77.636 | 1.00 | 60.00 |
| ATOM | 2335 | CD1 | LEU | 243 | 59.643 | 31.616 | 77.513 | 1.00 | 60.00 |
| ATOM | 2336 | CD2 | LEU | 243 | 60.879 | 33.743 | 76.813 | 1.00 | 60.00 |
| ATOM | 2337 | C | LEU | 243 | 57.575 | 33.816 | 79.591 | 1.00 | 60.00 |
| ATOM | 2338 | O | LEU | 243 | 57.890 | 34.978 | 79.848 | 1.00 | 60.00 |
| ATOM | 2339 | N | MET | 244 | 57.507 | 32.862 | 80.533 | 1.00 | 60.00 |
| ATOM | 2341 | CA | MET | 244 | 57.791 | 33.161 | 81.903 | 1.00 | 60.00 |
| ATOM | 2342 | CB | MET | 244 | 57.482 | 31.989 | 82.850 | 1.00 | 60.00 |
| ATOM | 2343 | CG | MET | 244 | 55.997 | 31.625 | 82.878 | 1.00 | 60.00 |
| ATOM | 2344 | SD | MET | 244 | 54.903 | 32.969 | 83.429 | 1.00 | 60.00 |
| ATOM | 2345 | CE | MET | 244 | 55.431 | 32.907 | 85.165 | 1.00 | 60.00 |
| ATOM | 2346 | C | MET | 244 | 59.235 | 33.503 | 82.057 | 1.00 | 60.00 |
| ATOM | 2347 | O | MET | 244 | 59.576 | 34.511 | 82.673 | 1.00 | 60.00 |
| ATOM | 2348 | N | LEU | 245 | 60.134 | 32.684 | 81.481 | 1.00 | 60.00 |
| ATOM | 2350 | CA | LEU | 245 | 61.525 | 32.981 | 81.643 | 1.00 | 60.00 |
| ATOM | 2351 | CB | LEU | 245 | 62.469 | 31.955 | 80.994 | 1.00 | 60.00 |
| ATOM | 2352 | CG | LEU | 245 | 62.377 | 30.548 | 81.616 | 1.00 | 60.00 |
| ATOM | 2353 | CD1 | LEU | 245 | 63.367 | 29.579 | 80.947 | 1.00 | 60.00 |
| ATOM | 2354 | CD2 | LEU | 245 | 62.526 | 30.598 | 83.146 | 1.00 | 60.00 |
| ATOM | 2355 | C | LEU | 245 | 61.771 | 34.296 | 80.992 | 1.00 | 60.00 |
| ATOM | 2356 | O | LEU | 245 | 61.191 | 34.605 | 79.952 | 1.00 | 60.00 |
| ATOM | 2357 | N | TYR | 246 | 62.630 | 35.127 | 81.612 | 1.00 | 60.00 |
| ATOM | 2359 | CA | TYR | 246 | 62.896 | 36.400 | 81.021 | 1.00 | 60.00 |
| ATOM | 2360 | CB | TYR | 246 | 62.429 | 37.596 | 81.868 | 1.00 | 60.00 |
| ATOM | 2361 | CG | TYR | 246 | 60.948 | 37.506 | 81.992 | 1.00 | 60.00 |
| ATOM | 2362 | CD1 | TYR | 246 | 60.132 | 37.819 | 80.930 | 1.00 | 60.00 |
| ATOM | 2363 | CE1 | TYR | 246 | 58.765 | 37.758 | 81.055 | 1.00 | 60.00 |
| ATOM | 2364 | CD2 | TYR | 246 | 60.374 | 37.171 | 83.196 | 1.00 | 60.00 |
| ATOM | 2365 | CE2 | TYR | 246 | 59.008 | 37.115 | 83.331 | 1.00 | 60.00 |
| ATOM | 2366 | CZ | TYR | 246 | 58.200 | 37.401 | 82.257 | 1.00 | 60.00 |
| ATOM | 2367 | OH | TYR | 246 | 56.798 | 37.332 | 82.389 | 1.00 | 60.00 |
| ATOM | 2369 | C | TYR | 246 | 64.369 | 36.547 | 80.860 | 1.00 | 60.00 |
| ATOM | 2370 | O | TYR | 246 | 65.152 | 36.112 | 81.704 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2371 | N | ASN | 247 | 64.781 | 37.156 | 79.735 | 1.00 | 60.00 |
| ATOM | 2373 | CA | ASN | 247 | 66.166 | 37.413 | 79.494 | 1.00 | 60.00 |
| ATOM | 2374 | CB | ASN | 247 | 66.751 | 36.629 | 78.307 | 1.00 | 60.00 |
| ATOM | 2375 | CG | ASN | 247 | 66.747 | 35.150 | 78.654 | 1.00 | 60.00 |
| ATOM | 2376 | OD1 | ASN | 247 | 66.946 | 34.764 | 79.804 | 1.00 | 60.00 |
| ATOM | 2377 | ND2 | ASN | 247 | 66.512 | 34.291 | 77.626 | 1.00 | 60.00 |
| ATOM | 2380 | C | ASN | 247 | 66.194 | 38.845 | 79.091 | 1.00 | 60.00 |
| ATOM | 2381 | O | ASN | 247 | 65.156 | 39.427 | 78.784 | 1.00 | 60.00 |
| ATOM | 2382 | N | PRO | 248 | 67.343 | 39.452 | 79.108 | 1.00 | 60.00 |
| ATOM | 2383 | CD | PRO | 248 | 68.307 | 39.227 | 80.172 | 1.00 | 60.00 |
| ATOM | 2384 | CA | PRO | 248 | 67.376 | 40.798 | 78.633 | 1.00 | 60.00 |
| ATOM | 2385 | CB | PRO | 248 | 68.694 | 41.391 | 79.120 | 1.00 | 60.00 |
| ATOM | 2386 | CG | PRO | 248 | 68.980 | 40.592 | 80.407 | 1.00 | 60.00 |
| ATOM | 2387 | C | PRO | 248 | 67.231 | 40.707 | 77.156 | 1.00 | 60.00 |
| ATOM | 2388 | O | PRO | 248 | 67.940 | 39.912 | 76.542 | 1.00 | 60.00 |
| ATOM | 2389 | N | THR | 249 | 66.324 | 41.498 | 76.561 | 1.00 | 60.00 |
| ATOM | 2391 | CA | THR | 249 | 66.157 | 41.376 | 75.148 | 1.00 | 60.00 |
| ATOM | 2392 | CB | THR | 249 | 64.766 | 40.988 | 74.743 | 1.00 | 60.00 |
| ATOM | 2393 | OG1 | THR | 249 | 63.842 | 41.988 | 75.145 | 1.00 | 60.00 |
| ATOM | 2395 | CG2 | THR | 249 | 64.419 | 39.645 | 75.406 | 1.00 | 60.00 |
| ATOM | 2396 | C | THR | 249 | 66.445 | 42.695 | 74.528 | 1.00 | 60.00 |
| ATOM | 2397 | O | THR | 249 | 65.998 | 43.736 | 75.007 | 1.00 | 60.00 |
| ATOM | 2398 | N | THR | 250 | 67.235 | 42.676 | 73.442 | 1.00 | 60.00 |
| ATOM | 2400 | CA | THR | 250 | 67.522 | 43.894 | 72.758 | 1.00 | 60.00 |
| ATOM | 2401 | CB | THR | 250 | 68.975 | 44.063 | 72.421 | 1.00 | 60.00 |
| ATOM | 2402 | OG1 | THR | 250 | 69.407 | 43.023 | 71.556 | 1.00 | 60.00 |
| ATOM | 2404 | CG2 | THR | 250 | 69.784 | 44.032 | 73.728 | 1.00 | 60.00 |
| ATOM | 2405 | C | THR | 250 | 66.755 | 43.825 | 71.483 | 1.00 | 60.00 |
| ATOM | 2406 | O | THR | 250 | 66.991 | 42.953 | 70.648 | 1.00 | 60.00 |
| ATOM | 2407 | N | TYR | 251 | 65.783 | 44.738 | 71.313 | 1.00 | 60.00 |
| ATOM | 2409 | CA | TYR | 251 | 65.019 | 44.726 | 70.106 | 1.00 | 60.00 |
| ATOM | 2410 | CB | TYR | 251 | 63.510 | 44.525 | 70.343 | 1.00 | 60.00 |
| ATOM | 2411 | CG | TYR | 251 | 62.876 | 44.130 | 69.052 | 1.00 | 60.00 |
| ATOM | 2412 | CD1 | TYR | 251 | 62.473 | 45.067 | 68.128 | 1.00 | 60.00 |
| ATOM | 2413 | CE1 | TYR | 251 | 61.893 | 44.675 | 66.943 | 1.00 | 60.00 |
| ATOM | 2414 | CD2 | TYR | 251 | 62.678 | 42.796 | 68.774 | 1.00 | 60.00 |
| ATOM | 2415 | CE2 | TYR | 251 | 62.096 | 42.398 | 67.594 | 1.00 | 60.00 |
| ATOM | 2416 | CZ | TYR | 251 | 61.705 | 43.340 | 66.674 | 1.00 | 60.00 |
| ATOM | 2417 | OH | TYR | 251 | 61.127 | 42.937 | 65.452 | 1.00 | 60.00 |
| ATOM | 2419 | C | TYR | 251 | 65.225 | 46.096 | 69.557 | 1.00 | 60.00 |
| ATOM | 2420 | O | TYR | 251 | 65.588 | 47.013 | 70.292 | 1.00 | 60.00 |
| ATOM | 2421 | N | GLN | 252 | 65.022 | 46.278 | 68.241 | 1.00 | 60.00 |
| ATOM | 2423 | CA | GLN | 252 | 65.242 | 47.587 | 67.707 | 1.00 | 60.00 |
| ATOM | 2424 | CB | GLN | 252 | 65.041 | 47.680 | 66.183 | 1.00 | 60.00 |
| ATOM | 2425 | CG | GLN | 252 | 63.628 | 47.363 | 65.693 | 1.00 | 60.00 |
| ATOM | 2426 | CD | GLN | 252 | 63.638 | 47.511 | 64.177 | 1.00 | 60.00 |
| ATOM | 2427 | OE1 | GLN | 252 | 62.715 | 47.085 | 63.482 | 1.00 | 60.00 |
| ATOM | 2428 | NE2 | GLN | 252 | 64.724 | 48.132 | 63.642 | 1.00 | 60.00 |
| ATOM | 2431 | C | GLN | 252 | 64.296 | 48.522 | 68.381 | 1.00 | 60.00 |
| ATOM | 2432 | O | GLN | 252 | 64.693 | 49.599 | 68.823 | 1.00 | 60.00 |
| ATOM | 2433 | N | MET | 253 | 63.015 | 48.127 | 68.504 | 1.00 | 60.00 |
| ATOM | 2435 | CA | MET | 253 | 62.094 | 49.001 | 69.160 | 1.00 | 60.00 |
| ATOM | 2436 | CB | MET | 253 | 60.612 | 48.669 | 68.906 | 1.00 | 60.00 |
| ATOM | 2437 | CG | MET | 253 | 60.179 | 48.955 | 67.466 | 1.00 | 60.00 |
| ATOM | 2438 | SD | MET | 253 | 58.436 | 48.593 | 67.098 | 1.00 | 60.00 |
| ATOM | 2439 | CE | MET | 253 | 58.658 | 46.796 | 66.971 | 1.00 | 60.00 |
| ATOM | 2440 | C | MET | 253 | 62.362 | 48.933 | 70.627 | 1.00 | 60.00 |
| ATOM | 2441 | O | MET | 253 | 63.037 | 48.023 | 71.106 | 1.00 | 60.00 |
| ATOM | 2442 | N | ASP | 254 | 61.848 | 49.926 | 71.374 | 1.00 | 60.00 |
| ATOM | 2444 | CA | ASP | 254 | 62.085 | 50.003 | 72.785 | 1.00 | 60.00 |
| ATOM | 2445 | CB | ASP | 254 | 61.483 | 51.270 | 73.416 | 1.00 | 60.00 |
| ATOM | 2446 | CG | ASP | 254 | 62.283 | 52.468 | 72.924 | 1.00 | 60.00 |
| ATOM | 2447 | OD1 | ASP | 254 | 61.662 | 53.540 | 72.691 | 1.00 | 60.00 |
| ATOM | 2448 | OD2 | ASP | 254 | 63.526 | 52.327 | 72.780 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| A | 2449 | C | ASP | 254 | 61.474 | 48.832 | 73.480 | 1.00 | 60.00 |
| ATOM | 2450 | O | ASP | 254 | 62.122 | 48.178 | 74.295 | 1.00 | 60.00 |
| ATOM | 2451 | N | VAL | 255 | 60.204 | 48.520 | 73.162 | 1.00 | 60.00 |
| ATOM | 2453 | CA | VAL | 255 | 59.561 | 47.442 | 73.852 | 1.00 | 60.00 |
| ATOM | 2454 | CB | VAL | 255 | 58.158 | 47.754 | 74.280 | 1.00 | 60.00 |
| ATOM | 2455 | CG1 | VAL | 255 | 57.299 | 47.953 | 73.020 | 1.00 | 60.00 |
| ATOM | 2456 | CG2 | VAL | 255 | 57.663 | 46.622 | 75.196 | 1.00 | 60.00 |
| ATOM | 2457 | C | VAL | 255 | 59.483 | 46.261 | 72.950 | 1.00 | 60.00 |
| ATOM | 2458 | O | VAL | 255 | 59.474 | 46.394 | 71.727 | 1.00 | 60.00 |
| ATOM | 2459 | N | ASN | 256 | 59.448 | 45.058 | 73.554 | 1.00 | 60.00 |
| ATOM | 2461 | CA | ASN | 256 | 59.348 | 43.852 | 72.791 | 1.00 | 60.00 |
| ATOM | 2462 | CB | ASN | 256 | 60.299 | 42.740 | 73.269 | 1.00 | 60.00 |
| ATOM | 2463 | CG | ASN | 256 | 60.098 | 41.520 | 72.379 | 1.00 | 60.00 |
| ATOM | 2464 | OD1 | ASN | 256 | 59.716 | 40.451 | 72.854 | 1.00 | 60.00 |
| ATOM | 2465 | ND2 | ASN | 256 | 60.362 | 41.679 | 71.055 | 1.00 | 60.00 |
| ATOM | 2468 | C | ASN | 256 | 57.957 | 43.344 | 72.963 | 1.00 | 60.00 |
| ATOM | 2469 | O | ASN | 256 | 57.392 | 43.371 | 74.055 | 1.00 | 60.00 |
| ATOM | 2470 | N | PRO | 257 | 57.384 | 42.907 | 71.879 | 1.00 | 60.00 |
| ATOM | 2471 | CD | PRO | 257 | 57.656 | 43.530 | 70.595 | 1.00 | 60.00 |
| ATOM | 2472 | CA | PRO | 257 | 56.058 | 42.359 | 71.940 | 1.00 | 60.00 |
| ATOM | 2473 | CB | PRO | 257 | 55.447 | 42.551 | 70.550 | 1.00 | 60.00 |
| ATOM | 2474 | CG | PRO | 257 | 56.643 | 42.882 | 69.640 | 1.00 | 60.00 |
| ATOM | 2475 | C | PRO | 257 | 56.163 | 40.932 | 72.357 | 1.00 | 60.00 |
| ATOM | 2476 | O | PRO | 257 | 57.229 | 40.343 | 72.188 | 1.00 | 60.00 |
| ATOM | 2477 | N | GLU | 258 | 55.084 | 40.355 | 72.921 | 1.00 | 60.00 |
| ATOM | 2479 | CA | GLU | 258 | 55.158 | 38.980 | 73.312 | 1.00 | 60.00 |
| ATOM | 2480 | CB | GLU | 258 | 56.103 | 38.741 | 74.504 | 1.00 | 60.00 |
| ATOM | 2481 | CG | GLU | 258 | 56.443 | 37.267 | 74.738 | 1.00 | 60.00 |
| ATOM | 2482 | CD | GLU | 258 | 57.436 | 36.838 | 73.666 | 1.00 | 60.00 |
| ATOM | 2483 | OE1 | GLU | 258 | 57.797 | 35.632 | 73.640 | 1.00 | 60.00 |
| ATOM | 2484 | OE2 | GLU | 258 | 57.850 | 37.712 | 72.857 | 1.00 | 60.00 |
| ATOM | 2485 | C | GLU | 258 | 53.785 | 38.555 | 73.725 | 1.00 | 60.00 |
| ATOM | 2486 | O | GLU | 258 | 52.822 | 39.305 | 73.579 | 1.00 | 60.00 |
| ATOM | 2487 | N | GLY | 259 | 53.662 | 37.318 | 74.242 | 1.00 | 60.00 |
| ATOM | 2489 | CA | GLY | 259 | 52.390 | 36.839 | 74.696 | 1.00 | 60.00 |
| ATOM | 2490 | C | GLY | 259 | 51.626 | 36.312 | 73.529 | 1.00 | 60.00 |
| ATOM | 2491 | O | GLY | 259 | 50.441 | 36.003 | 73.639 | 1.00 | 60.00 |
| ATOM | 2492 | N | LYS | 260 | 52.295 | 36.197 | 72.369 | 1.00 | 60.00 |
| ATOM | 2494 | CA | LYS | 260 | 51.630 | 35.712 | 71.199 | 1.00 | 60.00 |
| ATOM | 2495 | CB | LYS | 260 | 52.164 | 36.371 | 69.917 | 1.00 | 60.00 |
| ATOM | 2496 | CG | LYS | 260 | 53.689 | 36.306 | 69.792 | 1.00 | 60.00 |
| ATOM | 2497 | CD | LYS | 260 | 54.221 | 36.659 | 68.401 | 1.00 | 60.00 |
| ATOM | 2498 | CE | LYS | 260 | 54.298 | 35.459 | 67.454 | 1.00 | 60.00 |
| ATOM | 2499 | NZ | LYS | 260 | 52.941 | 35.089 | 66.995 | 1.00 | 60.00 |
| ATOM | 2503 | C | LYS | 260 | 51.855 | 34.239 | 71.090 | 1.00 | 60.00 |
| ATOM | 2504 | O | LYS | 260 | 52.807 | 33.792 | 70.452 | 1.00 | 60.00 |
| ATOM | 2505 | N | TYR | 261 | 50.981 | 33.433 | 71.727 | 1.00 | 40.00 |
| ATOM | 2507 | CA | TYR | 261 | 51.160 | 32.018 | 71.623 | 1.00 | 40.00 |
| ATOM | 2508 | CB | TYR | 261 | 51.545 | 31.368 | 72.964 | 1.00 | 40.00 |
| ATOM | 2509 | CG | TYR | 261 | 52.847 | 31.929 | 73.425 | 1.00 | 40.00 |
| ATOM | 2510 | CD1 | TYR | 261 | 54.032 | 31.338 | 73.054 | 1.00 | 40.00 |
| ATOM | 2511 | CE1 | TYR | 261 | 55.236 | 31.845 | 73.479 | 1.00 | 40.00 |
| ATOM | 2512 | CD2 | TYR | 261 | 52.884 | 33.038 | 74.239 | 1.00 | 40.00 |
| ATOM | 2513 | CE2 | TYR | 261 | 54.086 | 33.545 | 74.676 | 1.00 | 40.00 |
| ATOM | 2514 | CZ | TYR | 261 | 55.263 | 32.950 | 74.294 | 1.00 | 40.00 |
| ATOM | 2515 | OH | TYR | 261 | 56.497 | 33.472 | 74.737 | 1.00 | 40.00 |
| ATOM | 2517 | C | TYR | 261 | 49.844 | 31.408 | 71.265 | 1.00 | 40.00 |
| ATOM | 2518 | O | TYR | 261 | 48.937 | 31.398 | 72.092 | 1.00 | 40.00 |
| ATOM | 2519 | N | SER | 262 | 49.703 | 30.888 | 70.027 | 1.00 | 20.00 |
| ATOM | 2521 | CA | SER | 262 | 48.521 | 30.173 | 69.622 | 1.00 | 20.00 |
| ATOM | 2522 | CB | SER | 262 | 47.244 | 31.027 | 69.481 | 1.00 | 20.00 |
| ATOM | 2523 | OG | SER | 262 | 46.751 | 31.449 | 70.744 | 1.00 | 20.00 |
| ATOM | 2525 | C | SER | 262 | 48.809 | 29.661 | 68.248 | 1.00 | 20.00 |
| ATOM | 2526 | O | SER | 262 | 48.879 | 30.438 | 67.297 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2527 | N | PHE | 263 | 49.007 | 28.337 | 68.103 | 1.00 | 20.00 |
| ATOM | 2529 | CA | PHE | 263 | 49.269 | 27.813 | 66.796 | 1.00 | 20.00 |
| ATOM | 2530 | CB | PHE | 263 | 50.756 | 27.487 | 66.589 | 1.00 | 20.00 |
| ATOM | 2531 | CG | PHE | 263 | 51.541 | 28.737 | 66.794 | 1.00 | 20.00 |
| ATOM | 2532 | CD1 | PHE | 263 | 51.722 | 29.238 | 68.063 | 1.00 | 20.00 |
| ATOM | 2533 | CD2 | PHE | 263 | 52.221 | 29.322 | 65.751 | 1.00 | 20.00 |
| ATOM | 2534 | CE1 | PHE | 263 | 52.514 | 30.340 | 68.283 | 1.00 | 20.00 |
| ATOM | 2535 | CE2 | PHE | 263 | 53.032 | 30.412 | 65.967 | 1.00 | 20.00 |
| ATOM | 2536 | CZ | PHE | 263 | 53.171 | 30.932 | 67.232 | 1.00 | 20.00 |
| ATOM | 2537 | C | PHE | 263 | 48.550 | 26.503 | 66.726 | 1.00 | 20.00 |
| ATOM | 2538 | O | PHE | 263 | 48.960 | 25.536 | 67.364 | 1.00 | 20.00 |
| ATOM | 2539 | N | GLY | 264 | 47.473 | 26.411 | 65.928 | 1.00 | 20.00 |
| ATOM | 2541 | CA | GLY | 264 | 46.785 | 25.154 | 65.871 | 1.00 | 20.00 |
| ATOM | 2542 | C | GLY | 264 | 46.317 | 24.803 | 67.261 | 1.00 | 20.00 |
| ATOM | 2543 | O | GLY | 264 | 45.573 | 25.563 | 67.871 | 1.00 | 20.00 |
| ATOM | 2544 | N | ALA | 265 | 46.670 | 23.590 | 67.748 | 1.00 | 40.00 |
| ATOM | 2546 | CA | ALA | 265 | 46.384 | 23.068 | 69.064 | 1.00 | 40.00 |
| ATOM | 2547 | CB | ALA | 265 | 46.496 | 21.535 | 69.117 | 1.00 | 40.00 |
| ATOM | 2548 | C | ALA | 265 | 47.277 | 23.601 | 70.145 | 1.00 | 40.00 |
| ATOM | 2549 | O | ALA | 265 | 46.844 | 23.768 | 71.284 | 1.00 | 40.00 |
| ATOM | 2550 | N | THR | 266 | 48.561 | 23.860 | 69.823 | 1.00 | 20.00 |
| ATOM | 2552 | CA | THR | 266 | 49.516 | 24.233 | 70.830 | 1.00 | 20.00 |
| ATOM | 2553 | CB | THR | 266 | 50.712 | 23.327 | 70.865 | 1.00 | 20.00 |
| ATOM | 2554 | OG1 | THR | 266 | 51.422 | 23.408 | 69.638 | 1.00 | 20.00 |
| ATOM | 2556 | CG2 | THR | 266 | 50.227 | 21.887 | 71.101 | 1.00 | 20.00 |
| ATOM | 2557 | C | THR | 266 | 50.034 | 25.609 | 70.581 | 1.00 | 20.00 |
| ATOM | 2558 | O | THR | 266 | 49.552 | 26.321 | 69.703 | 1.00 | 20.00 |
| ATOM | 2559 | N | CYS | 267 | 51.024 | 26.035 | 71.393 | 1.00 | 20.00 |
| ATOM | 2561 | CA | CYS | 267 | 51.536 | 27.360 | 71.222 | 1.00 | 20.00 |
| ATOM | 2562 | CB | CYS | 267 | 51.243 | 28.267 | 72.417 | 1.00 | 20.00 |
| ATOM | 2563 | SG | CYS | 267 | 49.476 | 28.652 | 72.467 | 1.00 | 20.00 |
| ATOM | 2564 | C | CYS | 267 | 53.003 | 27.395 | 70.932 | 1.00 | 20.00 |
| ATOM | 2565 | O | CYS | 267 | 53.762 | 26.529 | 71.362 | 1.00 | 20.00 |
| ATOM | 2566 | N | VAL | 268 | 53.425 | 28.426 | 70.165 | 1.00 | 20.00 |
| ATOM | 2568 | CA | VAL | 268 | 54.797 | 28.586 | 69.772 | 1.00 | 20.00 |
| ATOM | 2569 | CB | VAL | 268 | 54.998 | 28.615 | 68.284 | 1.00 | 20.00 |
| ATOM | 2570 | CG1 | VAL | 268 | 56.489 | 28.857 | 67.997 | 1.00 | 20.00 |
| ATOM | 2571 | CG2 | VAL | 268 | 54.457 | 27.305 | 67.684 | 1.00 | 20.00 |
| ATOM | 2572 | C | VAL | 268 | 55.307 | 29.884 | 70.309 | 1.00 | 20.00 |
| ATOM | 2573 | O | VAL | 268 | 54.571 | 30.863 | 70.413 | 1.00 | 20.00 |
| ATOM | 2574 | N | LYS | 269 | 56.608 | 29.908 | 70.657 | 1.00 | 20.00 |
| ATOM | 2576 | CA | LYS | 269 | 57.239 | 31.058 | 71.241 | 1.00 | 20.00 |
| ATOM | 2577 | CB | LYS | 269 | 58.729 | 30.813 | 71.532 | 1.00 | 20.00 |
| ATOM | 2578 | CG | LYS | 269 | 59.426 | 31.973 | 72.242 | 1.00 | 20.00 |
| ATOM | 2579 | CD | LYS | 269 | 60.879 | 31.668 | 72.615 | 1.00 | 20.00 |
| ATOM | 2580 | CE | LYS | 269 | 61.061 | 30.346 | 73.364 | 1.00 | 20.00 |
| ATOM | 2581 | NZ | LYS | 269 | 62.503 | 30.064 | 73.551 | 1.00 | 20.00 |
| ATOM | 2585 | C | LYS | 269 | 57.176 | 32.209 | 70.297 | 1.00 | 20.00 |
| ATOM | 2586 | O | LYS | 269 | 56.810 | 33.318 | 70.685 | 1.00 | 20.00 |
| ATOM | 2587 | N | LYS | 270 | 57.522 | 31.969 | 69.019 | 1.00 | 20.00 |
| ATOM | 2589 | CA | LYS | 270 | 57.534 | 33.036 | 68.064 | 1.00 | 20.00 |
| ATOM | 2590 | CB | LYS | 270 | 58.948 | 33.382 | 67.571 | 1.00 | 20.00 |
| ATOM | 2591 | CG | LYS | 270 | 59.831 | 34.001 | 68.657 | 1.00 | 20.00 |
| ATOM | 2592 | CD | LYS | 270 | 61.323 | 33.973 | 68.323 | 1.00 | 20.00 |
| ATOM | 2593 | CE | LYS | 270 | 61.984 | 32.627 | 68.625 | 1.00 | 20.00 |
| ATOM | 2594 | NZ | LYS | 270 | 63.403 | 32.653 | 68.209 | 1.00 | 20.00 |
| ATOM | 2598 | C | LYS | 270 | 56.741 | 32.590 | 66.885 | 1.00 | 20.00 |
| ATOM | 2599 | O | LYS | 270 | 56.481 | 31.401 | 66.702 | 1.00 | 20.00 |
| ATOM | 2600 | N | CYS | 271 | 56.320 | 33.559 | 66.057 | 1.00 | 20.00 |
| ATOM | 2602 | CA | CYS | 271 | 55.524 | 33.261 | 64.908 | 1.00 | 20.00 |
| ATOM | 2603 | CB | CYS | 271 | 54.812 | 34.532 | 64.403 | 1.00 | 20.00 |
| ATOM | 2604 | SG | CYS | 271 | 53.495 | 34.290 | 63.178 | 1.00 | 20.00 |
| ATOM | 2605 | C | CYS | 271 | 56.458 | 32.726 | 63.869 | 1.00 | 20.00 |
| ATOM | 2606 | O | CYS | 271 | 57.559 | 33.242 | 63.686 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2607 | N | PRO | 272 | 56.054 | 31.683 | 63.193 | 1.00 | 20.00 |
| ATOM | 2608 | CD | PRO | 272 | 55.163 | 30.698 | 63.778 | 1.00 | 20.00 |
| ATOM | 2609 | CA | PRO | 272 | 56.883 | 31.103 | 62.177 | 1.00 | 20.00 |
| ATOM | 2610 | CB | PRO | 272 | 56.289 | 29.725 | 61.870 | 1.00 | 20.00 |
| ATOM | 2611 | CG | PRO | 272 | 54.955 | 29.688 | 62.639 | 1.00 | 20.00 |
| ATOM | 2612 | C | PRO | 272 | 56.936 | 32.042 | 61.023 | 1.00 | 20.00 |
| ATOM | 2613 | O | PRO | 272 | 56.040 | 32.873 | 60.891 | 1.00 | 20.00 |
| ATOM | 2614 | N | ARG | 273 | 57.979 | 31.943 | 60.181 | 1.00 | 20.00 |
| ATOM | 2616 | CA | ARG | 273 | 58.097 | 32.887 | 59.115 | 1.00 | 20.00 |
| ATOM | 2617 | CB | ARG | 273 | 59.407 | 32.762 | 58.313 | 1.00 | 20.00 |
| ATOM | 2618 | CG | ARG | 273 | 60.640 | 33.020 | 59.185 | 1.00 | 20.00 |
| ATOM | 2619 | CD | ARG | 273 | 61.938 | 33.257 | 58.409 | 1.00 | 20.00 |
| ATOM | 2620 | NE | ARG | 273 | 62.116 | 34.733 | 58.287 | 1.00 | 20.00 |
| ATOM | 2622 | CZ | ARG | 273 | 63.314 | 35.307 | 58.603 | 1.00 | 20.00 |
| ATOM | 2623 | NH1 | ARG | 273 | 64.351 | 34.532 | 59.035 | 1.00 | 20.00 |
| ATOM | 2626 | NH2 | ARG | 273 | 63.471 | 36.660 | 58.499 | 1.00 | 20.00 |
| ATOM | 2629 | C | ARG | 273 | 56.932 | 32.755 | 58.192 | 1.00 | 20.00 |
| ATOM | 2630 | O | ARG | 273 | 56.339 | 31.685 | 58.064 | 1.00 | 20.00 |
| ATOM | 2631 | N | ASN | 274 | 56.580 | 33.873 | 57.527 | 1.00 | 20.00 |
| ATOM | 2633 | CA | ASN | 274 | 55.465 | 33.937 | 56.628 | 1.00 | 20.00 |
| ATOM | 2634 | CB | ASN | 274 | 55.474 | 32.817 | 55.574 | 1.00 | 20.00 |
| ATOM | 2635 | CG | ASN | 274 | 56.592 | 33.129 | 54.587 | 1.00 | 20.00 |
| ATOM | 2636 | OD1 | ASN | 274 | 56.601 | 34.187 | 53.960 | 1.00 | 20.00 |
| ATOM | 2637 | ND2 | ASN | 274 | 57.566 | 32.189 | 54.450 | 1.00 | 20.00 |
| ATOM | 2640 | C | ASN | 274 | 54.178 | 33.873 | 57.388 | 1.00 | 20.00 |
| ATOM | 2641 | O | ASN | 274 | 53.123 | 33.612 | 56.812 | 1.00 | 20.00 |
| ATOM | 2642 | N | TYR | 275 | 54.234 | 34.130 | 58.709 | 1.00 | 20.00 |
| ATOM | 2644 | CA | TYR | 275 | 53.047 | 34.163 | 59.516 | 1.00 | 20.00 |
| ATOM | 2645 | CB | TYR | 275 | 52.918 | 32.988 | 60.503 | 1.00 | 20.00 |
| ATOM | 2646 | CG | TYR | 275 | 52.806 | 31.721 | 59.728 | 1.00 | 20.00 |
| ATOM | 2647 | CD1 | TYR | 275 | 53.939 | 31.105 | 59.253 | 1.00 | 20.00 |
| ATOM | 2648 | CE1 | TYR | 275 | 53.860 | 29.914 | 58.570 | 1.00 | 20.00 |
| ATOM | 2649 | CD2 | TYR | 275 | 51.588 | 31.112 | 59.535 | 1.00 | 20.00 |
| ATOM | 2650 | CE2 | TYR | 275 | 51.502 | 29.919 | 58.855 | 1.00 | 20.00 |
| ATOM | 2651 | CZ | TYR | 275 | 52.639 | 29.321 | 58.367 | 1.00 | 20.00 |
| ATOM | 2652 | OH | TYR | 275 | 52.555 | 28.099 | 57.668 | 1.00 | 20.00 |
| ATOM | 2654 | C | TYR | 275 | 53.176 | 35.407 | 60.339 | 1.00 | 20.00 |
| ATOM | 2655 | O | TYR | 275 | 54.285 | 35.859 | 60.621 | 1.00 | 20.00 |
| ATOM | 2656 | N | VAL | 276 | 52.038 | 36.005 | 60.741 | 1.00 | 20.00 |
| ATOM | 2658 | CA | VAL | 276 | 52.083 | 37.215 | 61.510 | 1.00 | 20.00 |
| ATOM | 2659 | CB | VAL | 276 | 51.371 | 38.363 | 60.858 | 1.00 | 20.00 |
| ATOM | 2660 | CG1 | VAL | 276 | 52.076 | 38.692 | 59.532 | 1.00 | 20.00 |
| ATOM | 2661 | CG2 | VAL | 276 | 49.884 | 37.996 | 60.703 | 1.00 | 20.00 |
| ATOM | 2662 | C | VAL | 276 | 51.393 | 36.980 | 62.815 | 1.00 | 20.00 |
| ATOM | 2663 | O | VAL | 276 | 50.633 | 36.025 | 62.967 | 1.00 | 20.00 |
| ATOM | 2664 | N | VAL | 277 | 51.665 | 37.850 | 63.808 | 1.00 | 20.00 |
| ATOM | 2666 | CA | VAL | 277 | 51.031 | 37.704 | 65.084 | 1.00 | 20.00 |
| ATOM | 2667 | CB | VAL | 277 | 51.935 | 38.005 | 66.244 | 1.00 | 20.00 |
| ATOM | 2668 | CG1 | VAL | 277 | 52.485 | 39.435 | 66.102 | 1.00 | 20.00 |
| ATOM | 2669 | CG2 | VAL | 277 | 51.138 | 37.780 | 67.538 | 1.00 | 20.00 |
| ATOM | 2670 | C | VAL | 277 | 49.878 | 38.649 | 65.131 | 1.00 | 20.00 |
| ATOM | 2671 | O | VAL | 277 | 50.037 | 39.853 | 64.942 | 1.00 | 20.00 |
| ATOM | 2672 | N | THR | 278 | 48.669 | 38.111 | 65.380 | 1.00 | 20.00 |
| ATOM | 2674 | CA | THR | 278 | 47.500 | 38.934 | 65.383 | 1.00 | 20.00 |
| ATOM | 2675 | CB | THR | 278 | 46.485 | 38.508 | 64.363 | 1.00 | 20.00 |
| ATOM | 2676 | OG1 | THR | 278 | 45.427 | 39.452 | 64.293 | 1.00 | 20.00 |
| ATOM | 2678 | CG2 | THR | 278 | 45.941 | 37.126 | 64.761 | 1.00 | 20.00 |
| ATOM | 2679 | C | THR | 278 | 46.832 | 38.866 | 66.713 | 1.00 | 20.00 |
| ATOM | 2680 | O | THR | 278 | 46.770 | 37.811 | 67.342 | 1.00 | 20.00 |
| ATOM | 2681 | N | ASP | 279 | 46.315 | 40.023 | 67.166 | 1.00 | 20.00 |
| ATOM | 2683 | CA | ASP | 279 | 45.606 | 40.114 | 68.405 | 1.00 | 20.00 |
| ATOM | 2684 | CB | ASP | 279 | 44.241 | 39.407 | 68.379 | 1.00 | 20.00 |
| ATOM | 2685 | CG | ASP | 279 | 43.322 | 40.199 | 67.462 | 1.00 | 20.00 |
| ATOM | 2686 | OD1 | ASP | 279 | 42.154 | 39.763 | 67.277 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2687 | OD2 | ASP | 279 | 43.775 | 41.249 | 66.933 | 1.00 | 20.00 |
| ATOM | 2688 | C | ASP | 279 | 46.411 | 39.511 | 69.499 | 1.00 | 20.00 |
| ATOM | 2689 | O | ASP | 279 | 45.855 | 38.829 | 70.358 | 1.00 | 20.00 |
| ATOM | 2690 | N | HIS | 280 | 47.734 | 39.785 | 69.489 | 1.00 | 20.00 |
| ATOM | 2692 | CA | HIS | 280 | 48.681 | 39.334 | 70.470 | 1.00 | 20.00 |
| ATOM | 2693 | CB | HIS | 280 | 48.754 | 40.258 | 71.699 | 1.00 | 20.00 |
| ATOM | 2694 | CG | HIS | 280 | 49.135 | 41.666 | 71.348 | 1.00 | 20.00 |
| ATOM | 2695 | CD2 | HIS | 280 | 48.349 | 42.719 | 70.991 | 1.00 | 20.00 |
| ATOM | 2696 | ND1 | HIS | 280 | 50.429 | 42.135 | 71.310 | 1.00 | 20.00 |
| ATOM | 2698 | CE1 | HIS | 280 | 50.362 | 43.439 | 70.939 | 1.00 | 20.00 |
| ATOM | 2699 | NE2 | HIS | 280 | 49.120 | 43.838 | 70.734 | 1.00 | 20.00 |
| ATOM | 2701 | C | HIS | 280 | 48.366 | 37.953 | 70.952 | 1.00 | 20.00 |
| ATOM | 2702 | O | HIS | 280 | 47.580 | 37.776 | 71.881 | 1.00 | 20.00 |
| ATOM | 2703 | N | GLY | 281 | 48.995 | 36.923 | 70.355 | 1.00 | 20.00 |
| ATOM | 2705 | CA | GLY | 281 | 48.682 | 35.604 | 70.816 | 1.00 | 20.00 |
| ATOM | 2706 | C | GLY | 281 | 48.423 | 34.647 | 69.699 | 1.00 | 20.00 |
| ATOM | 2707 | O | GLY | 281 | 48.690 | 33.456 | 69.844 | 1.00 | 20.00 |
| ATOM | 2708 | N | SER | 282 | 47.885 | 35.107 | 68.558 | 1.00 | 20.00 |
| ATOM | 2710 | CA | SER | 282 | 47.678 | 34.134 | 67.527 | 1.00 | 20.00 |
| ATOM | 2711 | CB | SER | 282 | 46.238 | 34.105 | 66.986 | 1.00 | 20.00 |
| ATOM | 2712 | OG | SER | 282 | 45.340 | 33.698 | 68.009 | 1.00 | 20.00 |
| ATOM | 2714 | C | SER | 282 | 48.580 | 34.438 | 66.380 | 1.00 | 20.00 |
| ATOM | 2715 | O | SER | 282 | 48.556 | 35.531 | 65.817 | 1.00 | 20.00 |
| ATOM | 2716 | N | CYS | 283 | 49.418 | 33.454 | 66.015 | 1.00 | 20.00 |
| ATOM | 2718 | CA | CYS | 283 | 50.301 | 33.582 | 64.897 | 1.00 | 20.00 |
| ATOM | 2719 | CB | CYS | 283 | 51.643 | 32.884 | 65.166 | 1.00 | 20.00 |
| ATOM | 2720 | SG | CYS | 283 | 52.649 | 32.524 | 63.700 | 1.00 | 20.00 |
| ATOM | 2721 | C | CYS | 283 | 49.600 | 32.877 | 63.794 | 1.00 | 20.00 |
| ATOM | 2722 | O | CYS | 283 | 49.413 | 31.660 | 63.829 | 1.00 | 20.00 |
| ATOM | 2723 | N | VAL | 284 | 49.168 | 33.651 | 62.786 | 1.00 | 20.00 |
| ATOM | 2725 | CA | VAL | 284 | 48.455 | 33.081 | 61.690 | 1.00 | 20.00 |
| ATOM | 2726 | CB | VAL | 284 | 47.049 | 33.602 | 61.572 | 1.00 | 20.00 |
| ATOM | 2727 | CG1 | VAL | 284 | 46.360 | 32.936 | 60.368 | 1.00 | 20.00 |
| ATOM | 2728 | CG2 | VAL | 284 | 46.329 | 33.358 | 62.910 | 1.00 | 20.00 |
| ATOM | 2729 | C | VAL | 284 | 49.198 | 33.470 | 60.457 | 1.00 | 20.00 |
| ATOM | 2730 | O | VAL | 284 | 49.960 | 34.435 | 60.453 | 1.00 | 20.00 |
| ATOM | 2731 | N | ARG | 285 | 48.992 | 32.705 | 59.373 | 1.00 | 20.00 |
| ATOM | 2733 | CA | ARG | 285 | 49.660 | 32.950 | 58.131 | 1.00 | 20.00 |
| ATOM | 2734 | CB | ARG | 285 | 49.252 | 31.937 | 57.047 | 1.00 | 20.00 |
| ATOM | 2735 | CG | ARG | 285 | 49.876 | 32.202 | 55.676 | 1.00 | 20.00 |
| ATOM | 2736 | CD | ARG | 285 | 49.454 | 31.184 | 54.614 | 1.00 | 20.00 |
| ATOM | 2737 | NE | ARG | 285 | 49.985 | 31.653 | 53.304 | 1.00 | 20.00 |
| ATOM | 2739 | CZ | ARG | 285 | 50.013 | 30.806 | 52.234 | 1.00 | 20.00 |
| ATOM | 2740 | NH1 | ARG | 285 | 49.586 | 29.517 | 52.373 | 1.00 | 20.00 |
| ATOM | 2743 | NH2 | ARG | 285 | 50.465 | 31.249 | 51.025 | 1.00 | 20.00 |
| ATOM | 2746 | C | ARG | 285 | 49.296 | 34.308 | 57.634 | 1.00 | 20.00 |
| ATOM | 2747 | O | ARG | 285 | 50.145 | 35.029 | 57.112 | 1.00 | 20.00 |
| ATOM | 2748 | N | ALA | 286 | 48.017 | 34.702 | 57.781 | 1.00 | 20.00 |
| ATOM | 2750 | CA | ALA | 286 | 47.642 | 35.980 | 57.256 | 1.00 | 20.00 |
| ATOM | 2751 | CB | ALA | 286 | 46.727 | 35.885 | 56.023 | 1.00 | 20.00 |
| ATOM | 2752 | C | ALA | 286 | 46.913 | 36.796 | 58.272 | 1.00 | 20.00 |
| ATOM | 2753 | O | ALA | 286 | 46.410 | 36.290 | 59.274 | 1.00 | 20.00 |
| ATOM | 2754 | N | CYS | 287 | 46.855 | 38.113 | 58.006 | 1.00 | 20.00 |
| ATOM | 2756 | CA | CYS | 287 | 46.200 | 39.081 | 58.834 | 1.00 | 20.00 |
| ATOM | 2757 | CB | CYS | 287 | 46.299 | 40.502 | 58.269 | 1.00 | 20.00 |
| ATOM | 2758 | SG | CYS | 287 | 47.899 | 41.323 | 58.457 | 1.00 | 20.00 |
| ATOM | 2759 | C | CYS | 287 | 44.735 | 38.810 | 58.806 | 1.00 | 20.00 |
| ATOM | 2760 | O | CYS | 287 | 44.243 | 38.046 | 57.978 | 1.00 | 20.00 |
| ATOM | 2761 | N | GLY | 288 | 43.999 | 39.446 | 59.736 | 1.00 | 20.00 |
| ATOM | 2763 | CA | GLY | 288 | 42.575 | 39.329 | 59.719 | 1.00 | 20.00 |
| ATOM | 2764 | C | GLY | 288 | 42.177 | 40.174 | 58.549 | 1.00 | 20.00 |
| ATOM | 2765 | O | GLY | 288 | 42.978 | 40.948 | 58.028 | 1.00 | 20.00 |
| ATOM | 2766 | N | ALA | 289 | 40.906 | 40.066 | 58.126 | 1.00 | 20.00 |
| ATOM | 2768 | CA | ALA | 289 | 40.434 | 40.735 | 56.947 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2769 | CB | ALA | 289 | 38.904 | 40.669 | 56.805 | 1.00 | 20.00 |
| ATOM | 2770 | C | ALA | 289 | 40.821 | 42.180 | 56.864 | 1.00 | 20.00 |
| ATOM | 2771 | O | ALA | 289 | 41.713 | 42.542 | 56.102 | 1.00 | 20.00 |
| ATOM | 2772 | N | ASP | 290 | 40.173 | 43.038 | 57.672 | 1.00 | 20.00 |
| ATOM | 2774 | CA | ASP | 290 | 40.355 | 44.462 | 57.620 | 1.00 | 20.00 |
| ATOM | 2775 | CB | ASP | 290 | 39.461 | 45.210 | 58.627 | 1.00 | 20.00 |
| ATOM | 2776 | CG | ASP | 290 | 38.016 | 45.075 | 58.168 | 1.00 | 20.00 |
| ATOM | 2777 | OD1 | ASP | 290 | 37.104 | 45.361 | 58.989 | 1.00 | 20.00 |
| ATOM | 2778 | OD2 | ASP | 290 | 37.805 | 44.683 | 56.989 | 1.00 | 20.00 |
| ATOM | 2779 | C | ASP | 290 | 41.768 | 44.843 | 57.925 | 1.00 | 20.00 |
| ATOM | 2780 | O | ASP | 290 | 42.165 | 45.983 | 57.690 | 1.00 | 20.00 |
| ATOM | 2781 | N | SER | 291 | 42.566 | 43.912 | 58.480 | 1.00 | 20.00 |
| ATOM | 2783 | CA | SER | 291 | 43.899 | 44.283 | 58.856 | 1.00 | 20.00 |
| ATOM | 2784 | CB | SER | 291 | 44.405 | 43.492 | 60.073 | 1.00 | 20.00 |
| ATOM | 2785 | OG | SER | 291 | 43.597 | 43.771 | 61.208 | 1.00 | 20.00 |
| ATOM | 2787 | C | SER | 291 | 44.881 | 44.081 | 57.740 | 1.00 | 20.00 |
| ATOM | 2788 | O | SER | 291 | 44.771 | 43.144 | 56.950 | 1.00 | 20.00 |
| ATOM | 2789 | N | TYR | 292 | 45.879 | 44.989 | 57.659 | 1.00 | 20.00 |
| ATOM | 2791 | CA | TYR | 292 | 46.897 | 44.937 | 56.647 | 1.00 | 20.00 |
| ATOM | 2792 | CB | TYR | 292 | 46.871 | 46.172 | 55.725 | 1.00 | 20.00 |
| ATOM | 2793 | CG | TYR | 292 | 47.867 | 45.995 | 54.629 | 1.00 | 20.00 |
| ATOM | 2794 | CD1 | TYR | 292 | 47.565 | 45.202 | 53.546 | 1.00 | 20.00 |
| ATOM | 2795 | CE1 | TYR | 292 | 48.422 | 45.115 | 52.473 | 1.00 | 20.00 |
| ATOM | 2796 | CD2 | TYR | 292 | 49.031 | 46.728 | 54.606 | 1.00 | 20.00 |
| ATOM | 2797 | CE2 | TYR | 292 | 49.894 | 46.647 | 53.537 | 1.00 | 20.00 |
| ATOM | 2798 | CZ | TYR | 292 | 49.588 | 45.840 | 52.468 | 1.00 | 20.00 |
| ATOM | 2799 | OH | TYR | 292 | 50.460 | 45.771 | 51.361 | 1.00 | 20.00 |
| ATOM | 2801 | C | TYR | 292 | 48.208 | 44.923 | 57.372 | 1.00 | 20.00 |
| ATOM | 2802 | O | TYR | 292 | 48.360 | 45.564 | 58.410 | 1.00 | 20.00 |
| ATOM | 2803 | N | GLU | 293 | 49.196 | 44.173 | 56.847 | 1.00 | 20.00 |
| ATOM | 2805 | CA | GLU | 293 | 50.458 | 44.087 | 57.520 | 1.00 | 20.00 |
| ATOM | 2806 | CB | GLU | 293 | 51.435 | 43.108 | 56.848 | 1.00 | 20.00 |
| ATOM | 2807 | CG | GLU | 293 | 50.980 | 41.649 | 56.936 | 1.00 | 20.00 |
| ATOM | 2808 | CD | GLU | 293 | 51.942 | 40.809 | 56.112 | 1.00 | 20.00 |
| ATOM | 2809 | OE1 | GLU | 293 | 52.657 | 41.402 | 55.261 | 1.00 | 20.00 |
| ATOM | 2810 | OE2 | GLU | 293 | 51.973 | 39.565 | 56.314 | 1.00 | 20.00 |
| ATOM | 2811 | C | GLU | 293 | 51.059 | 45.450 | 57.503 | 1.00 | 20.00 |
| ATOM | 2812 | O | GLU | 293 | 50.902 | 46.201 | 56.544 | 1.00 | 20.00 |
| ATOM | 2813 | N | MET | 294 | 51.769 | 45.811 | 58.585 | 1.00 | 20.00 |
| ATOM | 2815 | CA | MET | 294 | 52.333 | 47.123 | 58.656 | 1.00 | 20.00 |
| ATOM | 2816 | CB | MET | 294 | 53.112 | 47.352 | 59.960 | 1.00 | 20.00 |
| ATOM | 2817 | CG | MET | 294 | 53.536 | 48.804 | 60.183 | 1.00 | 20.00 |
| ATOM | 2818 | SD | MET | 294 | 54.296 | 49.118 | 61.805 | 1.00 | 20.00 |
| ATOM | 2819 | CE | MET | 294 | 52.763 | 48.901 | 62.755 | 1.00 | 20.00 |
| ATOM | 2820 | C | MET | 294 | 53.277 | 47.263 | 57.509 | 1.00 | 20.00 |
| ATOM | 2821 | O | MET | 294 | 53.288 | 48.282 | 56.821 | 1.00 | 20.00 |
| ATOM | 2822 | N | GLU | 295 | 54.092 | 46.223 | 57.261 | 1.00 | 20.00 |
| ATOM | 2824 | CA | GLU | 295 | 55.006 | 46.271 | 56.159 | 1.00 | 20.00 |
| ATOM | 2825 | CB | GLU | 295 | 56.483 | 46.382 | 56.567 | 1.00 | 20.00 |
| ATOM | 2826 | CG | GLU | 295 | 57.405 | 46.649 | 55.377 | 1.00 | 20.00 |
| ATOM | 2827 | CD | GLU | 295 | 57.090 | 48.047 | 54.861 | 1.00 | 20.00 |
| ATOM | 2828 | OE1 | GLU | 295 | 56.385 | 48.150 | 53.821 | 1.00 | 20.00 |
| ATOM | 2829 | OE2 | GLU | 295 | 57.540 | 49.030 | 55.507 | 1.00 | 20.00 |
| ATOM | 2830 | C | GLU | 295 | 54.838 | 44.988 | 55.415 | 1.00 | 20.00 |
| ATOM | 2831 | O | GLU | 295 | 54.121 | 44.094 | 55.859 | 1.00 | 20.00 |
| ATOM | 2832 | N | GLU | 296 | 55.490 | 44.866 | 54.244 | 1.00 | 20.00 |
| ATOM | 2834 | CA | GLU | 296 | 55.329 | 43.665 | 53.482 | 1.00 | 20.00 |
| ATOM | 2835 | CB | GLU | 296 | 56.167 | 43.632 | 52.194 | 1.00 | 20.00 |
| ATOM | 2836 | CG | GLU | 296 | 55.849 | 42.419 | 51.316 | 1.00 | 20.00 |
| ATOM | 2837 | CD | GLU | 296 | 56.724 | 42.489 | 50.075 | 1.00 | 20.00 |
| ATOM | 2838 | OE1 | GLU | 296 | 57.977 | 42.466 | 50.233 | 1.00 | 20.00 |
| ATOM | 2839 | OE2 | GLU | 296 | 56.157 | 42.569 | 48.956 | 1.00 | 20.00 |
| ATOM | 2840 | C | GLU | 296 | 55.774 | 42.521 | 54.331 | 1.00 | 20.00 |
| ATOM | 2841 | O | GLU | 296 | 55.066 | 41.525 | 54.468 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2842 | N | ASP | 297 | 56.970 | 42.635 | 54.934 | 1.00 | 40.00 |
| ATOM | 2844 | CA | ASP | 297 | 57.418 | 41.570 | 55.776 | 1.00 | 40.00 |
| ATOM | 2845 | CB | ASP | 297 | 58.374 | 40.583 | 55.082 | 1.00 | 40.00 |
| ATOM | 2846 | CG | ASP | 297 | 59.628 | 41.336 | 54.661 | 1.00 | 40.00 |
| ATOM | 2847 | OD1 | ASP | 297 | 59.573 | 42.593 | 54.589 | 1.00 | 40.00 |
| ATOM | 2848 | OD2 | ASP | 297 | 60.659 | 40.661 | 54.401 | 1.00 | 40.00 |
| ATOM | 2849 | C | ASP | 297 | 58.159 | 42.195 | 56.906 | 1.00 | 40.00 |
| ATOM | 2850 | O | ASP | 297 | 58.306 | 43.413 | 56.973 | 1.00 | 40.00 |
| ATOM | 2851 | N | GLY | 298 | 58.621 | 41.360 | 57.852 | 1.00 | 40.00 |
| ATOM | 2853 | CA | GLY | 298 | 59.365 | 41.874 | 58.959 | 1.00 | 40.00 |
| ATOM | 2854 | C | GLY | 298 | 58.382 | 42.422 | 59.933 | 1.00 | 40.00 |
| ATOM | 2855 | O | GLY | 298 | 58.728 | 42.737 | 61.071 | 1.00 | 40.00 |
| ATOM | 2856 | N | VAL | 299 | 57.114 | 42.556 | 59.503 | 1.00 | 40.00 |
| ATOM | 2858 | CA | VAL | 299 | 56.137 | 43.068 | 60.407 | 1.00 | 40.00 |
| ATOM | 2859 | CB | VAL | 299 | 55.345 | 44.214 | 59.844 | 1.00 | 40.00 |
| ATOM | 2860 | CG1 | VAL | 299 | 56.292 | 45.415 | 59.674 | 1.00 | 40.00 |
| ATOM | 2861 | CG2 | VAL | 299 | 54.702 | 43.772 | 58.520 | 1.00 | 40.00 |
| ATOM | 2862 | C | VAL | 299 | 55.203 | 41.967 | 60.792 | 1.00 | 40.00 |
| ATOM | 2863 | O | VAL | 299 | 54.374 | 41.506 | 60.010 | 1.00 | 40.00 |
| ATOM | 2864 | N | ARG | 300 | 55.364 | 41.477 | 62.030 | 1.00 | 20.00 |
| ATOM | 2866 | CA | ARG | 300 | 54.469 | 40.486 | 62.537 | 1.00 | 20.00 |
| ATOM | 2867 | CB | ARG | 300 | 54.946 | 39.864 | 63.859 | 1.00 | 20.00 |
| ATOM | 2868 | CG | ARG | 300 | 56.093 | 38.870 | 63.662 | 1.00 | 20.00 |
| ATOM | 2869 | CD | ARG | 300 | 57.381 | 39.499 | 63.127 | 1.00 | 20.00 |
| ATOM | 2870 | NE | ARG | 300 | 58.323 | 38.383 | 62.831 | 1.00 | 20.00 |
| ATOM | 2872 | CZ | ARG | 300 | 59.632 | 38.640 | 62.541 | 1.00 | 20.00 |
| ATOM | 2873 | NH1 | ARG | 300 | 60.101 | 39.922 | 62.564 | 1.00 | 20.00 |
| ATOM | 2876 | NH2 | ARG | 300 | 60.473 | 37.612 | 62.228 | 1.00 | 20.00 |
| ATOM | 2879 | C | ARG | 300 | 53.169 | 41.175 | 62.776 | 1.00 | 20.00 |
| ATOM | 2880 | O | ARG | 300 | 52.100 | 40.597 | 62.589 | 1.00 | 20.00 |
| ATOM | 2881 | N | LYS | 301 | 53.247 | 42.451 | 63.196 | 1.00 | 20.00 |
| ATOM | 2883 | CA | LYS | 301 | 52.083 | 43.220 | 63.518 | 1.00 | 20.00 |
| ATOM | 2884 | CB | LYS | 301 | 52.403 | 44.615 | 64.088 | 1.00 | 20.00 |
| ATOM | 2885 | CG | LYS | 301 | 52.891 | 44.624 | 65.538 | 1.00 | 20.00 |
| ATOM | 2886 | CD | LYS | 301 | 51.836 | 44.146 | 66.537 | 1.00 | 20.00 |
| ATOM | 2887 | CE | LYS | 301 | 52.219 | 44.386 | 68.000 | 1.00 | 20.00 |
| ATOM | 2888 | NZ | LYS | 301 | 51.988 | 45.804 | 68.357 | 1.00 | 20.00 |
| ATOM | 2892 | C | LYS | 301 | 51.244 | 43.447 | 62.312 | 1.00 | 20.00 |
| ATOM | 2893 | O | LYS | 301 | 51.740 | 43.586 | 61.194 | 1.00 | 20.00 |
| ATOM | 2894 | N | CYS | 302 | 49.917 | 43.473 | 62.525 | 1.00 | 20.00 |
| ATOM | 2896 | CA | CYS | 302 | 49.042 | 43.769 | 61.443 | 1.00 | 20.00 |
| ATOM | 2897 | CB | CYS | 302 | 48.002 | 42.684 | 61.152 | 1.00 | 20.00 |
| ATOM | 2898 | SG | CYS | 302 | 47.330 | 42.959 | 59.499 | 1.00 | 20.00 |
| ATOM | 2899 | C | CYS | 302 | 48.314 | 44.990 | 61.905 | 1.00 | 20.00 |
| ATOM | 2900 | O | CYS | 302 | 48.036 | 45.132 | 63.095 | 1.00 | 20.00 |
| ATOM | 2901 | N | LYS | 303 | 48.003 | 45.922 | 60.983 | 1.00 | 20.00 |
| ATOM | 2903 | CA | LYS | 303 | 47.356 | 47.128 | 61.407 | 1.00 | 20.00 |
| ATOM | 2904 | CB | LYS | 303 | 48.242 | 48.374 | 61.231 | 1.00 | 20.00 |
| ATOM | 2905 | CG | LYS | 303 | 48.792 | 48.550 | 59.816 | 1.00 | 20.00 |
| ATOM | 2906 | CD | LYS | 303 | 49.481 | 49.898 | 59.594 | 1.00 | 20.00 |
| ATOM | 2907 | CE | LYS | 303 | 50.235 | 49.985 | 58.265 | 1.00 | 20.00 |
| ATOM | 2908 | NZ | LYS | 303 | 50.850 | 51.323 | 58.116 | 1.00 | 20.00 |
| ATOM | 2912 | C | LYS | 303 | 46.078 | 47.329 | 60.654 | 1.00 | 20.00 |
| ATOM | 2913 | O | LYS | 303 | 45.879 | 46.778 | 59.574 | 1.00 | 20.00 |
| ATOM | 2914 | N | LYS | 304 | 45.169 | 48.129 | 61.247 | 1.00 | 20.00 |
| ATOM | 2916 | CA | LYS | 304 | 43.869 | 48.421 | 60.711 | 1.00 | 20.00 |
| ATOM | 2917 | CB | LYS | 304 | 43.032 | 49.283 | 61.672 | 1.00 | 20.00 |
| ATOM | 2918 | CG | LYS | 304 | 41.630 | 49.631 | 61.174 | 1.00 | 20.00 |
| ATOM | 2919 | CD | LYS | 304 | 40.782 | 50.330 | 62.240 | 1.00 | 20.00 |
| ATOM | 2920 | CE | LYS | 304 | 39.436 | 50.849 | 61.726 | 1.00 | 20.00 |
| ATOM | 2921 | NZ | LYS | 304 | 38.423 | 49.771 | 61.774 | 1.00 | 20.00 |
| ATOM | 2925 | C | LYS | 304 | 43.997 | 49.190 | 59.438 | 1.00 | 20.00 |
| ATOM | 2926 | O | LYS | 304 | 44.899 | 50.012 | 59.285 | 1.00 | 20.00 |
| ATOM | 2927 | N | CYS | 305 | 43.095 | 48.927 | 58.472 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 2929 | CA | CYS | 305 | 43.164 | 49.684 | 57.260 | 1.00 | 20.00 |
| ATOM | 2930 | CB | CYS | 305 | 43.302 | 48.823 | 55.985 | 1.00 | 20.00 |
| ATOM | 2931 | SG | CYS | 305 | 41.828 | 47.850 | 55.573 | 1.00 | 20.00 |
| ATOM | 2932 | C | CYS | 305 | 41.923 | 50.512 | 57.184 | 1.00 | 20.00 |
| ATOM | 2933 | O | CYS | 305 | 40.806 | 49.999 | 57.237 | 1.00 | 20.00 |
| ATOM | 2934 | N | GLU | 306 | 42.086 | 51.844 | 57.077 | 1.00 | 20.00 |
| ATOM | 2936 | CA | GLU | 306 | 40.918 | 52.669 | 57.024 | 1.00 | 20.00 |
| ATOM | 2937 | CB | GLU | 306 | 41.217 | 54.178 | 57.005 | 1.00 | 20.00 |
| ATOM | 2938 | CG | GLU | 306 | 41.776 | 54.707 | 58.328 | 1.00 | 20.00 |
| ATOM | 2939 | CD | GLU | 306 | 40.654 | 54.677 | 59.357 | 1.00 | 20.00 |
| ATOM | 2940 | OE1 | GLU | 306 | 39.574 | 54.114 | 59.035 | 1.00 | 20.00 |
| ATOM | 2941 | OE2 | GLU | 306 | 40.861 | 55.214 | 60.478 | 1.00 | 20.00 |
| ATOM | 2942 | C | GLU | 306 | 40.199 | 52.336 | 55.763 | 1.00 | 20.00 |
| ATOM | 2943 | O | GLU | 306 | 40.732 | 52.501 | 54.667 | 1.00 | 20.00 |
| ATOM | 2944 | N | GLY | 307 | 38.949 | 51.857 | 55.896 | 1.00 | 20.00 |
| ATOM | 2946 | CA | GLY | 307 | 38.172 | 51.522 | 54.741 | 1.00 | 20.00 |
| ATOM | 2947 | C | GLY | 307 | 38.614 | 50.195 | 54.230 | 1.00 | 20.00 |
| ATOM | 2948 | O | GLY | 307 | 39.196 | 49.387 | 54.951 | 1.00 | 20.00 |
| ATOM | 2949 | N | PRO | 308 | 38.336 | 49.955 | 52.980 | 1.00 | 20.00 |
| ATOM | 2950 | CD | PRO | 308 | 37.118 | 50.454 | 52.364 | 1.00 | 20.00 |
| ATOM | 2951 | CA | PRO | 308 | 38.754 | 48.713 | 52.409 | 1.00 | 20.00 |
| ATOM | 2952 | CB | PRO | 308 | 38.045 | 48.614 | 51.062 | 1.00 | 20.00 |
| ATOM | 2953 | CG | PRO | 308 | 36.747 | 49.414 | 51.290 | 1.00 | 20.00 |
| ATOM | 2954 | C | PRO | 308 | 40.240 | 48.737 | 52.352 | 1.00 | 20.00 |
| ATOM | 2955 | O | PRO | 308 | 40.805 | 49.802 | 52.108 | 1.00 | 20.00 |
| ATOM | 2956 | N | CYS | 309 | 40.901 | 47.588 | 52.578 | 1.00 | 20.00 |
| ATOM | 2958 | CA | CYS | 309 | 42.329 | 47.631 | 52.587 | 1.00 | 20.00 |
| ATOM | 2959 | CB | CYS | 309 | 43.015 | 46.386 | 53.168 | 1.00 | 20.00 |
| ATOM | 2960 | SG | CYS | 309 | 42.556 | 46.072 | 54.897 | 1.00 | 20.00 |
| ATOM | 2961 | C | CYS | 309 | 42.789 | 47.801 | 51.182 | 1.00 | 20.00 |
| ATOM | 2962 | O | CYS | 309 | 42.104 | 47.406 | 50.240 | 1.00 | 20.00 |
| ATOM | 2963 | N | ARG | 310 | 43.972 | 48.421 | 51.015 | 1.00 | 20.00 |
| ATOM | 2965 | CA | ARG | 310 | 44.498 | 48.664 | 49.709 | 1.00 | 20.00 |
| ATOM | 2966 | CB | ARG | 310 | 45.726 | 49.594 | 49.699 | 1.00 | 20.00 |
| ATOM | 2967 | CG | ARG | 310 | 45.450 | 51.064 | 50.032 | 1.00 | 20.00 |
| ATOM | 2968 | CD | ARG | 310 | 44.884 | 51.307 | 51.433 | 1.00 | 20.00 |
| ATOM | 2969 | NE | ARG | 310 | 43.403 | 51.169 | 51.346 | 1.00 | 20.00 |
| ATOM | 2971 | CZ | ARG | 310 | 42.641 | 52.281 | 51.125 | 1.00 | 20.00 |
| ATOM | 2972 | NH1 | ARG | 310 | 43.236 | 53.506 | 51.036 | 1.00 | 20.00 |
| ATOM | 2975 | NH2 | ARG | 310 | 41.286 | 52.172 | 50.995 | 1.00 | 20.00 |
| ATOM | 2978 | C | ARG | 310 | 44.942 | 47.373 | 49.114 | 1.00 | 20.00 |
| ATOM | 2979 | O | ARG | 310 | 45.419 | 46.479 | 49.811 | 1.00 | 20.00 |
| ATOM | 2980 | N | LYS | 311 | 44.756 | 47.247 | 47.787 | 1.00 | 20.00 |
| ATOM | 2982 | CA | LYS | 311 | 45.195 | 46.091 | 47.069 | 1.00 | 20.00 |
| ATOM | 2983 | CB | LYS | 311 | 44.107 | 45.021 | 46.887 | 1.00 | 20.00 |

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|------|----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 3 | N | CYS | 313 | 54.063 | 9.046 | 61.837 | 1.00 | 40.00 |
| ATOM | 5 | CA | CYS | 313 | 54.050 | 8.871 | 60.363 | 1.00 | 40.00 |
| ATOM | 6 | CB | CYS | 313 | 53.300 | 7.570 | 60.029 | 1.00 | 40.00 |
| ATOM | 7 | SG | CYS | 313 | 54.210 | 6.124 | 60.659 | 1.00 | 40.00 |
| ATOM | 8 | C | CYS | 313 | 53.390 | 10.060 | 59.715 | 1.00 | 40.00 |
| ATOM | 9 | O | CYS | 313 | 52.565 | 10.713 | 60.344 | 1.00 | 40.00 |
| ATOM | 10 | N | ASN | 314 | 53.749 | 10.398 | 58.452 | 1.00 | 40.00 |
| ATOM | 12 | CA | ASN | 314 | 53.183 | 11.550 | 57.785 | 1.00 | 40.00 |
| ATOM | 13 | CB | ASN | 314 | 54.130 | 12.176 | 56.746 | 1.00 | 40.00 |
| ATOM | 14 | CG | ASN | 314 | 54.433 | 11.136 | 55.678 | 1.00 | 40.00 |
| ATOM | 15 | OD1 | ASN | 314 | 54.238 | 9.938 | 55.880 | 1.00 | 40.00 |
| ATOM | 16 | ND2 | ASN | 314 | 54.937 | 11.606 | 54.505 | 1.00 | 40.00 |
| ATOM | 19 | C | ASN | 314 | 51.911 | 11.161 | 57.091 | 1.00 | 40.00 |
| ATOM | 20 | O | ASN | 314 | 51.514 | 9.999 | 57.138 | 1.00 | 40.00 |
| ATOM | 21 | N | GLY | 315 | 51.235 | 12.143 | 56.442 | 1.00 | 20.00 |
| ATOM | 23 | CA | GLY | 315 | 49.998 | 11.903 | 55.745 | 1.00 | 20.00 |
| ATOM | 24 | C | GLY | 315 | 50.241 | 10.746 | 54.839 | 1.00 | 20.00 |
| ATOM | 25 | O | GLY | 315 | 51.148 | 10.775 | 54.010 | 1.00 | 20.00 |
| ATOM | 26 | N | ILE | 316 | 49.421 | 9.689 | 54.982 | 1.00 | 20.00 |
| ATOM | 28 | CA | ILE | 316 | 49.654 | 8.506 | 54.212 | 1.00 | 20.00 |
| ATOM | 29 | CB | ILE | 316 | 49.701 | 7.266 | 55.060 | 1.00 | 20.00 |
| ATOM | 30 | CG2 | ILE | 316 | 49.810 | 6.043 | 54.134 | 1.00 | 20.00 |
| ATOM | 31 | CG1 | ILE | 316 | 50.840 | 7.372 | 56.089 | 1.00 | 20.00 |
| ATOM | 32 | CD1 | ILE | 316 | 50.774 | 6.314 | 57.189 | 1.00 | 20.00 |
| ATOM | 33 | C | ILE | 316 | 48.554 | 8.324 | 53.222 | 1.00 | 20.00 |
| ATOM | 34 | O | ILE | 316 | 47.383 | 8.559 | 53.518 | 1.00 | 20.00 |
| ATOM | 35 | N | GLY | 317 | 48.916 | 7.913 | 51.992 | 1.00 | 20.00 |
| ATOM | 37 | CA | GLY | 317 | 47.898 | 7.677 | 51.018 | 1.00 | 20.00 |
| ATOM | 38 | C | GLY | 317 | 48.178 | 6.350 | 50.401 | 1.00 | 20.00 |
| ATOM | 39 | O | GLY | 317 | 48.942 | 6.247 | 49.443 | 1.00 | 20.00 |
| ATOM | 40 | N | ILE | 318 | 47.543 | 5.290 | 50.933 | 1.00 | 20.00 |
| ATOM | 42 | CA | ILE | 318 | 47.728 | 3.986 | 50.371 | 1.00 | 20.00 |
| ATOM | 43 | CB | ILE | 318 | 47.758 | 2.881 | 51.385 | 1.00 | 20.00 |
| ATOM | 44 | CG2 | ILE | 318 | 49.016 | 3.053 | 52.249 | 1.00 | 20.00 |
| ATOM | 45 | CG1 | ILE | 318 | 46.447 | 2.831 | 52.178 | 1.00 | 20.00 |
| ATOM | 46 | CD1 | ILE | 318 | 46.354 | 1.602 | 53.078 | 1.00 | 20.00 |
| ATOM | 47 | C | ILE | 318 | 46.595 | 3.745 | 49.429 | 1.00 | 20.00 |
| ATOM | 48 | O | ILE | 318 | 45.691 | 4.571 | 49.319 | 1.00 | 20.00 |
| ATOM | 49 | N | GLY | 319 | 46.626 | 2.611 | 48.699 | 1.00 | 40.00 |
| ATOM | 51 | CA | GLY | 319 | 45.557 | 2.342 | 47.782 | 1.00 | 40.00 |
| ATOM | 52 | C | GLY | 319 | 46.137 | 2.189 | 46.416 | 1.00 | 40.00 |
| ATOM | 53 | O | GLY | 319 | 46.896 | 1.261 | 46.142 | 1.00 | 40.00 |
| ATOM | 54 | N | GLU | 320 | 45.781 | 3.123 | 45.516 | 1.00 | 40.00 |
| ATOM | 56 | CA | GLU | 320 | 46.284 | 3.084 | 44.178 | 1.00 | 40.00 |
| ATOM | 57 | CB | GLU | 320 | 47.797 | 3.351 | 44.098 | 1.00 | 40.00 |
| ATOM | 58 | CG | GLU | 320 | 48.335 | 3.435 | 42.670 | 1.00 | 40.00 |
| ATOM | 59 | CD | GLU | 320 | 49.826 | 3.732 | 42.752 | 1.00 | 40.00 |
| ATOM | 60 | OE1 | GLU | 320 | 50.461 | 3.873 | 41.673 | 1.00 | 40.00 |
| ATOM | 61 | OE2 | GLU | 320 | 50.350 | 3.829 | 43.894 | 1.00 | 40.00 |
| ATOM | 62 | C | GLU | 320 | 46.002 | 1.771 | 43.534 | 1.00 | 40.00 |
| ATOM | 63 | O | GLU | 320 | 46.780 | 0.825 | 43.637 | 1.00 | 40.00 |
| ATOM | 64 | N | PHE | 321 | 44.840 | 1.688 | 42.861 | 1.00 | 60.00 |
| ATOM | 66 | CA | PHE | 321 | 44.481 | 0.492 | 42.166 | 1.00 | 60.00 |
| ATOM | 67 | CB | PHE | 321 | 43.051 | 0.531 | 41.598 | 1.00 | 60.00 |
| ATOM | 68 | CG | PHE | 321 | 42.809 | -0.724 | 40.830 | 1.00 | 60.00 |
| ATOM | 69 | CD1 | PHE | 321 | 43.173 | -0.813 | 39.504 | 1.00 | 60.00 |
| ATOM | 70 | CD2 | PHE | 321 | 42.188 | -1.800 | 41.418 | 1.00 | 60.00 |
| ATOM | 71 | CE1 | PHE | 321 | 42.944 | -1.958 | 38.780 | 1.00 | 60.00 |
| ATOM | 72 | CE2 | PHE | 321 | 41.947 | -2.947 | 40.697 | 1.00 | 60.00 |
| ATOM | 73 | CZ | PHE | 321 | 42.326 | -3.028 | 39.379 | 1.00 | 60.00 |
| ATOM | 74 | C | PHE | 321 | 45.414 | 0.351 | 41.014 | 1.00 | 60.00 |
| ATOM | 75 | O | PHE | 321 | 45.223 | 0.969 | 39.967 | 1.00 | 60.00 |
| ATOM | 76 | N | LYS | 322 | 46.461 | -0.474 | 41.190 | 1.00 | 60.00 |
| ATOM | 78 | CA | LYS | 322 | 47.379 | -0.713 | 40.121 | 1.00 | 60.00 |

Figure 7

| | | | | | | | | | |
|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| A | 79 | CB | LYS | 322 | 48.815 | -0.252 | 40.428 | 1.00 | 60.00 |
| ATOM | 80 | CG | LYS | 322 | 49.803 | -0.503 | 39.286 | 1.00 | 60.00 |
| ATOM | 81 | CD | LYS | 322 | 49.579 | 0.390 | 38.062 | 1.00 | 60.00 |
| W | 82 | CE | LYS | 322 | 48.513 | -0.125 | 37.093 | 1.00 | 60.00 |
| ATOM | 83 | NZ | LYS | 322 | 48.375 | 0.808 | 35.950 | 1.00 | 60.00 |
| ATOM | 87 | C | LYS | 322 | 47.420 | -2.191 | 39.932 | 1.00 | 60.00 |
| ATOM | 88 | O | LYS | 322 | 47.746 | -2.936 | 40.855 | 1.00 | 60.00 |
| ATOM | 89 | N | ASP | 323 | 47.051 | -2.658 | 38.726 | 1.00 | 60.00 |
| ATOM | 91 | CA | ASP | 323 | 47.099 | -4.062 | 38.456 | 1.00 | 60.00 |
| ATOM | 92 | CB | ASP | 323 | 46.397 | -4.458 | 37.143 | 1.00 | 60.00 |
| ATOM | 93 | CG | ASP | 323 | 47.108 | -3.784 | 35.978 | 1.00 | 60.00 |
| ATOM | 94 | OD1 | ASP | 323 | 47.322 | -4.469 | 34.942 | 1.00 | 60.00 |
| ATOM | 95 | OD2 | ASP | 323 | 47.433 | -2.574 | 36.104 | 1.00 | 60.00 |
| ATOM | 96 | C | ASP | 323 | 48.538 | -4.441 | 38.350 | 1.00 | 60.00 |
| ATOM | 97 | O | ASP | 323 | 48.930 | -5.553 | 38.698 | 1.00 | 60.00 |
| ATOM | 98 | N | SER | 324 | 49.371 | -3.492 | 37.882 | 1.00 | 60.00 |
| ATOM | 100 | CA | SER | 324 | 50.760 | -3.756 | 37.658 | 1.00 | 60.00 |
| ATOM | 101 | CB | SER | 324 | 51.544 | -2.494 | 37.259 | 1.00 | 60.00 |
| ATOM | 102 | OG | SER | 324 | 51.058 | -1.985 | 36.026 | 1.00 | 60.00 |
| ATOM | 104 | C | SER | 324 | 51.395 | -4.290 | 38.899 | 1.00 | 60.00 |
| ATOM | 105 | O | SER | 324 | 52.008 | -5.357 | 38.874 | 1.00 | 60.00 |
| ATOM | 106 | N | LEU | 325 | 51.255 | -3.578 | 40.032 | 1.00 | 60.00 |
| ATOM | 108 | CA | LEU | 325 | 51.896 | -4.060 | 41.219 | 1.00 | 60.00 |
| ATOM | 109 | CB | LEU | 325 | 51.804 | -3.116 | 42.430 | 1.00 | 60.00 |
| ATOM | 110 | CG | LEU | 325 | 52.625 | -1.823 | 42.267 | 1.00 | 60.00 |
| ATOM | 111 | CD1 | LEU | 325 | 52.077 | -0.948 | 41.128 | 1.00 | 60.00 |
| ATOM | 112 | CD2 | LEU | 325 | 52.755 | -1.070 | 43.601 | 1.00 | 60.00 |
| ATOM | 113 | C | LEU | 325 | 51.288 | -5.362 | 41.603 | 1.00 | 60.00 |
| ATOM | 114 | O | LEU | 325 | 50.220 | -5.735 | 41.119 | 1.00 | 60.00 |
| ATOM | 115 | N | SER | 326 | 51.986 | -6.105 | 42.482 | 1.00 | 60.00 |
| ATOM | 117 | CA | SER | 326 | 51.499 | -7.384 | 42.897 | 1.00 | 60.00 |
| ATOM | 118 | CB | SER | 326 | 52.451 | -8.095 | 43.874 | 1.00 | 60.00 |
| ATOM | 119 | OG | SER | 326 | 51.915 | -9.354 | 44.250 | 1.00 | 60.00 |
| ATOM | 121 | C | SER | 326 | 50.202 | -7.174 | 43.599 | 1.00 | 60.00 |
| ATOM | 122 | O | SER | 326 | 49.180 | -7.743 | 43.219 | 1.00 | 60.00 |
| ATOM | 123 | N | ILE | 327 | 50.204 | -6.324 | 44.644 | 1.00 | 60.00 |
| ATOM | 125 | CA | ILE | 327 | 48.983 | -6.090 | 45.352 | 1.00 | 60.00 |
| ATOM | 126 | CB | ILE | 327 | 48.834 | -6.950 | 46.573 | 1.00 | 60.00 |
| ATOM | 127 | CG2 | ILE | 327 | 49.917 | -6.537 | 47.583 | 1.00 | 60.00 |
| ATOM | 128 | CG1 | ILE | 327 | 47.402 | -6.864 | 47.126 | 1.00 | 60.00 |
| ATOM | 129 | CD1 | ILE | 327 | 46.352 | -7.480 | 46.202 | 1.00 | 60.00 |
| ATOM | 130 | C | ILE | 327 | 48.969 | -4.668 | 45.802 | 1.00 | 60.00 |
| ATOM | 131 | O | ILE | 327 | 50.015 | -4.078 | 46.071 | 1.00 | 60.00 |
| ATOM | 132 | N | ASN | 328 | 47.762 | -4.072 | 45.865 | 1.00 | 40.00 |
| ATOM | 134 | CA | ASN | 328 | 47.611 | -2.726 | 46.322 | 1.00 | 40.00 |
| ATOM | 135 | CB | ASN | 328 | 46.295 | -2.093 | 45.841 | 1.00 | 40.00 |
| ATOM | 136 | CG | ASN | 328 | 46.384 | -1.981 | 44.323 | 1.00 | 40.00 |
| ATOM | 137 | OD1 | ASN | 328 | 47.466 | -1.791 | 43.771 | 1.00 | 40.00 |
| ATOM | 138 | ND2 | ASN | 328 | 45.223 | -2.111 | 43.626 | 1.00 | 40.00 |
| ATOM | 141 | C | ASN | 328 | 47.578 | -2.827 | 47.812 | 1.00 | 40.00 |
| ATOM | 142 | O | ASN | 328 | 47.893 | -1.878 | 48.529 | 1.00 | 40.00 |
| ATOM | 143 | N | ALA | 329 | 47.214 | -4.025 | 48.301 | 1.00 | 40.00 |
| ATOM | 145 | CA | ALA | 329 | 47.117 | -4.326 | 49.698 | 1.00 | 40.00 |
| ATOM | 146 | CB | ALA | 329 | 46.633 | -5.761 | 49.967 | 1.00 | 40.00 |
| ATOM | 147 | C | ALA | 329 | 48.482 | -4.197 | 50.290 | 1.00 | 40.00 |
| ATOM | 148 | O | ALA | 329 | 48.636 | -3.841 | 51.456 | 1.00 | 40.00 |
| ATOM | 149 | N | THR | 330 | 49.518 | -4.458 | 49.476 | 1.00 | 40.00 |
| ATOM | 151 | CA | THR | 330 | 50.871 | -4.441 | 49.946 | 1.00 | 40.00 |
| ATOM | 152 | CB | THR | 330 | 51.875 | -4.612 | 48.845 | 1.00 | 40.00 |
| ATOM | 153 | OG1 | THR | 330 | 53.174 | -4.807 | 49.385 | 1.00 | 40.00 |
| ATOM | 155 | CG2 | THR | 330 | 51.853 | -3.347 | 47.972 | 1.00 | 40.00 |
| ATOM | 156 | C | THR | 330 | 51.143 | -3.117 | 50.583 | 1.00 | 40.00 |
| ATOM | 157 | O | THR | 330 | 51.963 | -3.021 | 51.493 | 1.00 | 40.00 |
| ATOM | 158 | N | ASN | 331 | 50.459 | -2.059 | 50.112 | 1.00 | 40.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 160 | CA | ASN | 331 | 50.645 | -0.728 | 50.616 | 1.00 | 40.00 |
| ATOM | 161 | CB | ASN | 331 | 49.784 | 0.317 | 49.883 | 1.00 | 40.00 |
| ATOM | 162 | CG | ASN | 331 | 50.411 | 0.592 | 48.522 | 1.00 | 40.00 |
| ATOM | 163 | OD1 | ASN | 331 | 50.424 | -0.259 | 47.634 | 1.00 | 40.00 |
| ATOM | 164 | ND2 | ASN | 331 | 50.947 | 1.831 | 48.353 | 1.00 | 40.00 |
| ATOM | 167 | C | ASN | 331 | 50.311 | -0.634 | 52.079 | 1.00 | 40.00 |
| ATOM | 168 | O | ASN | 331 | 50.896 | 0.175 | 52.796 | 1.00 | 40.00 |
| ATOM | 169 | N | ILE | 332 | 49.370 | -1.468 | 52.558 | 1.00 | 40.00 |
| ATOM | 171 | CA | ILE | 332 | 48.883 | -1.467 | 53.915 | 1.00 | 40.00 |
| ATOM | 172 | CB | ILE | 332 | 47.753 | -2.450 | 54.108 | 1.00 | 40.00 |
| ATOM | 173 | CG2 | ILE | 332 | 47.465 | -2.606 | 55.611 | 1.00 | 40.00 |
| ATOM | 174 | CG1 | ILE | 332 | 46.510 | -1.984 | 53.324 | 1.00 | 40.00 |
| ATOM | 175 | CD1 | ILE | 332 | 46.687 | -1.946 | 51.808 | 1.00 | 40.00 |
| ATOM | 176 | C | ILE | 332 | 49.982 | -1.751 | 54.903 | 1.00 | 40.00 |
| ATOM | 177 | O | ILE | 332 | 49.872 | -1.399 | 56.076 | 1.00 | 40.00 |
| ATOM | 178 | N | LYS | 333 | 51.066 | -2.412 | 54.462 | 1.00 | 40.00 |
| ATOM | 180 | CA | LYS | 333 | 52.173 | -2.772 | 55.309 | 1.00 | 40.00 |
| ATOM | 181 | CB | LYS | 333 | 53.279 | -3.515 | 54.544 | 1.00 | 40.00 |
| ATOM | 182 | CG | LYS | 333 | 52.838 | -4.845 | 53.933 | 1.00 | 40.00 |
| ATOM | 183 | CD | LYS | 333 | 53.866 | -5.413 | 52.953 | 1.00 | 40.00 |
| ATOM | 184 | CE | LYS | 333 | 53.457 | -6.746 | 52.323 | 1.00 | 40.00 |
| ATOM | 185 | NZ | LYS | 333 | 54.529 | -7.228 | 51.422 | 1.00 | 40.00 |
| ATOM | 189 | C | LYS | 333 | 52.828 | -1.565 | 55.913 | 1.00 | 40.00 |
| ATOM | 190 | O | LYS | 333 | 53.348 | -1.628 | 57.025 | 1.00 | 40.00 |
| ATOM | 191 | N | HIS | 334 | 52.803 | -0.423 | 55.204 | 1.00 | 40.00 |
| ATOM | 193 | CA | HIS | 334 | 53.459 | 0.777 | 55.644 | 1.00 | 40.00 |
| ATOM | 194 | CB | HIS | 334 | 53.101 | 1.980 | 54.753 | 1.00 | 40.00 |
| ATOM | 195 | CG | HIS | 334 | 53.623 | 3.291 | 55.265 | 1.00 | 40.00 |
| ATOM | 196 | CD2 | HIS | 334 | 52.952 | 4.317 | 55.858 | 1.00 | 40.00 |
| ATOM | 197 | ND1 | HIS | 334 | 54.937 | 3.695 | 55.190 | 1.00 | 40.00 |
| ATOM | 199 | CE1 | HIS | 334 | 54.996 | 4.935 | 55.738 | 1.00 | 40.00 |
| ATOM | 200 | NE2 | HIS | 334 | 53.816 | 5.355 | 56.157 | 1.00 | 40.00 |
| ATOM | 202 | C | HIS | 334 | 53.016 | 1.117 | 57.030 | 1.00 | 40.00 |
| ATOM | 203 | O | HIS | 334 | 53.778 | 1.672 | 57.818 | 1.00 | 40.00 |
| ATOM | 204 | N | PHE | 335 | 51.753 | 0.791 | 57.336 | 1.00 | 40.00 |
| ATOM | 206 | CA | PHE | 335 | 51.061 | 1.055 | 58.562 | 1.00 | 40.00 |
| ATOM | 207 | CB | PHE | 335 | 49.554 | 0.799 | 58.431 | 1.00 | 40.00 |
| ATOM | 208 | CG | PHE | 335 | 49.102 | 1.681 | 57.320 | 1.00 | 40.00 |
| ATOM | 209 | CD1 | PHE | 335 | 48.896 | 1.164 | 56.062 | 1.00 | 40.00 |
| ATOM | 210 | CD2 | PHE | 335 | 49.140 | 3.047 | 57.469 | 1.00 | 40.00 |
| ATOM | 211 | CE1 | PHE | 335 | 48.627 | 1.983 | 54.990 | 1.00 | 40.00 |
| ATOM | 212 | CE2 | PHE | 335 | 48.902 | 3.873 | 56.397 | 1.00 | 40.00 |
| ATOM | 213 | CZ | PHE | 335 | 48.625 | 3.345 | 55.159 | 1.00 | 40.00 |
| ATOM | 214 | C | PHE | 335 | 51.559 | 0.283 | 59.744 | 1.00 | 40.00 |
| ATOM | 215 | O | PHE | 335 | 51.268 | 0.647 | 60.879 | 1.00 | 40.00 |
| ATOM | 216 | N | LYS | 336 | 52.301 | -0.815 | 59.536 | 1.00 | 40.00 |
| ATOM | 218 | CA | LYS | 336 | 52.650 | -1.655 | 60.647 | 1.00 | 40.00 |
| ATOM | 219 | CB | LYS | 336 | 53.554 | -2.830 | 60.237 | 1.00 | 40.00 |
| ATOM | 220 | CG | LYS | 336 | 52.800 | -3.964 | 59.540 | 1.00 | 40.00 |
| ATOM | 221 | CD | LYS | 336 | 51.765 | -4.630 | 60.450 | 1.00 | 40.00 |
| ATOM | 222 | CE | LYS | 336 | 50.988 | -5.769 | 59.788 | 1.00 | 40.00 |
| ATOM | 223 | NZ | LYS | 336 | 50.020 | -6.339 | 60.752 | 1.00 | 40.00 |
| ATOM | 227 | C | LYS | 336 | 53.325 | -0.951 | 61.793 | 1.00 | 40.00 |
| ATOM | 228 | O | LYS | 336 | 53.026 | -1.250 | 62.946 | 1.00 | 40.00 |
| ATOM | 229 | N | ASN | 337 | 54.284 | -0.045 | 61.530 | 1.00 | 40.00 |
| ATOM | 231 | CA | ASN | 337 | 54.995 | 0.629 | 62.589 | 1.00 | 40.00 |
| ATOM | 232 | CB | ASN | 337 | 56.335 | 1.211 | 62.109 | 1.00 | 40.00 |
| ATOM | 233 | CG | ASN | 337 | 57.267 | 0.038 | 61.842 | 1.00 | 40.00 |
| ATOM | 234 | OD1 | ASN | 337 | 57.310 | -0.920 | 62.613 | 1.00 | 40.00 |
| ATOM | 235 | ND2 | ASN | 337 | 58.031 | 0.106 | 60.719 | 1.00 | 40.00 |
| ATOM | 238 | C | ASN | 337 | 54.274 | 1.726 | 63.336 | 1.00 | 40.00 |
| ATOM | 239 | O | ASN | 337 | 54.441 | 1.867 | 64.546 | 1.00 | 40.00 |
| ATOM | 240 | N | CYS | 338 | 53.450 | 2.529 | 62.634 | 1.00 | 20.00 |
| ATOM | 242 | CA | CYS | 338 | 52.859 | 3.733 | 63.159 | 1.00 | 20.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| A | 243 | CB | CYS | 338 | 52.042 | 4.491 | 62.087 | 1.00 | 20.00 |
| ATOM | 244 | SG | CYS | 338 | 52.908 | 4.575 | 60.487 | 1.00 | 20.00 |
| ATOM | 245 | C | CYS | 338 | 51.966 | 3.576 | 64.354 | 1.00 | 20.00 |
| M | 246 | O | CYS | 338 | 50.994 | 2.823 | 64.335 | 1.00 | 20.00 |
| ATOM | 247 | N | THR | 339 | 52.356 | 4.224 | 65.473 | 1.00 | 20.00 |
| ATOM | 249 | CA | THR | 339 | 51.526 | 4.354 | 66.634 | 1.00 | 20.00 |
| ATOM | 250 | CB | THR | 339 | 52.332 | 4.553 | 67.880 | 1.00 | 20.00 |
| ATOM | 251 | OG1 | THR | 339 | 51.470 | 4.672 | 69.000 | 1.00 | 20.00 |
| ATOM | 253 | CG2 | THR | 339 | 53.197 | 5.812 | 67.719 | 1.00 | 20.00 |
| ATOM | 254 | C | THR | 339 | 50.613 | 5.531 | 66.451 | 1.00 | 20.00 |
| ATOM | 255 | O | THR | 339 | 49.437 | 5.490 | 66.809 | 1.00 | 20.00 |
| ATOM | 256 | N | SER | 340 | 51.146 | 6.642 | 65.898 | 1.00 | 20.00 |
| ATOM | 258 | CA | SER | 340 | 50.317 | 7.795 | 65.714 | 1.00 | 20.00 |
| ATOM | 259 | CB | SER | 340 | 50.454 | 8.820 | 66.856 | 1.00 | 20.00 |
| ATOM | 260 | OG | SER | 340 | 51.788 | 9.301 | 66.938 | 1.00 | 20.00 |
| ATOM | 262 | C | SER | 340 | 50.677 | 8.482 | 64.438 | 1.00 | 20.00 |
| ATOM | 263 | O | SER | 340 | 51.676 | 9.194 | 64.362 | 1.00 | 20.00 |
| ATOM | 264 | N | ILE | 341 | 49.850 | 8.318 | 63.390 | 1.00 | 20.00 |
| ATOM | 266 | CA | ILE | 341 | 50.200 | 8.984 | 62.177 | 1.00 | 20.00 |
| ATOM | 267 | CB | ILE | 341 | 49.518 | 8.470 | 60.942 | 1.00 | 20.00 |
| ATOM | 268 | CG2 | ILE | 341 | 50.047 | 7.067 | 60.638 | 1.00 | 20.00 |
| ATOM | 269 | CG1 | ILE | 341 | 47.995 | 8.562 | 61.072 | 1.00 | 20.00 |
| ATOM | 270 | CD1 | ILE | 341 | 47.273 | 8.284 | 59.755 | 1.00 | 20.00 |
| ATOM | 271 | C | ILE | 341 | 49.868 | 10.426 | 62.330 | 1.00 | 20.00 |
| ATOM | 272 | O | ILE | 341 | 48.711 | 10.792 | 62.521 | 1.00 | 20.00 |
| ATOM | 273 | N | SER | 342 | 50.901 | 11.287 | 62.273 | 1.00 | 20.00 |
| ATOM | 275 | CA | SER | 342 | 50.671 | 12.692 | 62.381 | 1.00 | 20.00 |
| ATOM | 276 | CB | SER | 342 | 51.889 | 13.483 | 62.888 | 1.00 | 20.00 |
| ATOM | 277 | OG | SER | 342 | 52.193 | 13.107 | 64.223 | 1.00 | 20.00 |
| ATOM | 279 | C | SER | 342 | 50.364 | 13.165 | 61.002 | 1.00 | 20.00 |
| ATOM | 280 | O | SER | 342 | 51.259 | 13.536 | 60.243 | 1.00 | 20.00 |
| ATOM | 281 | N | GLY | 343 | 49.065 | 13.173 | 60.654 | 1.00 | 20.00 |
| ATOM | 283 | CA | GLY | 343 | 48.661 | 13.571 | 59.341 | 1.00 | 20.00 |
| ATOM | 284 | C | GLY | 343 | 47.366 | 12.873 | 59.096 | 1.00 | 20.00 |
| ATOM | 285 | O | GLY | 343 | 46.609 | 12.606 | 60.026 | 1.00 | 20.00 |
| ATOM | 286 | N | ASP | 344 | 47.073 | 12.555 | 57.824 | 1.00 | 20.00 |
| ATOM | 288 | CA | ASP | 344 | 45.833 | 11.906 | 57.524 | 1.00 | 20.00 |
| ATOM | 289 | CB | ASP | 344 | 44.961 | 12.709 | 56.536 | 1.00 | 20.00 |
| ATOM | 290 | CG | ASP | 344 | 45.728 | 12.897 | 55.232 | 1.00 | 20.00 |
| ATOM | 291 | OD1 | ASP | 344 | 46.922 | 12.501 | 55.179 | 1.00 | 20.00 |
| ATOM | 292 | OD2 | ASP | 344 | 45.130 | 13.455 | 54.272 | 1.00 | 20.00 |
| ATOM | 293 | C | ASP | 344 | 46.100 | 10.563 | 56.933 | 1.00 | 20.00 |
| ATOM | 294 | O | ASP | 344 | 47.197 | 10.290 | 56.452 | 1.00 | 20.00 |
| ATOM | 295 | N | LEU | 345 | 45.098 | 9.664 | 56.999 | 1.00 | 20.00 |
| ATOM | 297 | CA | LEU | 345 | 45.262 | 8.362 | 56.427 | 1.00 | 20.00 |
| ATOM | 298 | CB | LEU | 345 | 45.064 | 7.222 | 57.438 | 1.00 | 20.00 |
| ATOM | 299 | CG | LEU | 345 | 45.234 | 5.831 | 56.810 | 1.00 | 20.00 |
| ATOM | 300 | CD1 | LEU | 345 | 46.611 | 5.704 | 56.157 | 1.00 | 20.00 |
| ATOM | 301 | CD2 | LEU | 345 | 44.967 | 4.716 | 57.834 | 1.00 | 20.00 |
| ATOM | 302 | C | LEU | 345 | 44.237 | 8.203 | 55.351 | 1.00 | 20.00 |
| ATOM | 303 | O | LEU | 345 | 43.061 | 8.494 | 55.558 | 1.00 | 20.00 |
| ATOM | 304 | N | HIS | 346 | 44.671 | 7.763 | 54.152 | 1.00 | 20.00 |
| ATOM | 306 | CA | HIS | 346 | 43.738 | 7.541 | 53.085 | 1.00 | 20.00 |
| ATOM | 307 | CB | HIS | 346 | 43.989 | 8.395 | 51.827 | 1.00 | 20.00 |
| ATOM | 308 | CG | HIS | 346 | 43.667 | 9.851 | 51.988 | 1.00 | 20.00 |
| ATOM | 309 | CD2 | HIS | 346 | 42.906 | 10.487 | 52.921 | 1.00 | 20.00 |
| ATOM | 310 | ND1 | HIS | 346 | 44.071 | 10.828 | 51.105 | 1.00 | 20.00 |
| ATOM | 312 | CE1 | HIS | 346 | 43.545 | 11.998 | 51.546 | 1.00 | 20.00 |
| ATOM | 313 | NE2 | HIS | 346 | 42.830 | 11.841 | 52.645 | 1.00 | 20.00 |
| ATOM | 315 | C | HIS | 346 | 43.890 | 6.122 | 52.650 | 1.00 | 20.00 |
| ATOM | 316 | O | HIS | 346 | 44.995 | 5.670 | 52.356 | 1.00 | 20.00 |
| ATOM | 317 | N | ILE | 347 | 42.778 | 5.366 | 52.619 | 1.00 | 20.00 |
| ATOM | 319 | CA | ILE | 347 | 42.884 | 4.018 | 52.151 | 1.00 | 20.00 |
| ATOM | 320 | CB | ILE | 347 | 42.422 | 3.010 | 53.159 | 1.00 | 20.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 321 | CG2 | ILE | 347 | 42.527 | 1.621 | 52.511 | 1.00 | 20.00 |
| ATOM | 322 | CG1 | ILE | 347 | 43.253 | 3.143 | 54.449 | 1.00 | 20.00 |
| ATOM | 323 | CD1 | ILE | 347 | 42.665 | 2.393 | 55.644 | 1.00 | 20.00 |
| ATOM | 324 | C | ILE | 347 | 42.000 | 3.938 | 50.952 | 1.00 | 20.00 |
| ATOM | 325 | O | ILE | 347 | 40.795 | 3.715 | 51.052 | 1.00 | 20.00 |
| ATOM | 326 | N | LEU | 348 | 42.607 | 4.094 | 49.766 | 1.00 | 20.00 |
| ATOM | 328 | CA | LEU | 348 | 41.882 | 4.138 | 48.533 | 1.00 | 20.00 |
| ATOM | 329 | CB | LEU | 348 | 42.700 | 4.845 | 47.444 | 1.00 | 20.00 |
| ATOM | 330 | CG | LEU | 348 | 43.043 | 6.285 | 47.877 | 1.00 | 20.00 |
| ATOM | 331 | CD1 | LEU | 348 | 43.859 | 7.034 | 46.817 | 1.00 | 20.00 |
| ATOM | 332 | CD2 | LEU | 348 | 41.778 | 7.053 | 48.295 | 1.00 | 20.00 |
| ATOM | 333 | C | LEU | 348 | 41.557 | 2.743 | 48.110 | 1.00 | 20.00 |
| ATOM | 334 | O | LEU | 348 | 41.948 | 1.769 | 48.753 | 1.00 | 20.00 |
| ATOM | 335 | N | PRO | 349 | 40.852 | 2.625 | 47.019 | 1.00 | 60.00 |
| ATOM | 336 | CD | PRO | 349 | 40.061 | 3.714 | 46.470 | 1.00 | 60.00 |
| ATOM | 337 | CA | PRO | 349 | 40.393 | 1.344 | 46.575 | 1.00 | 60.00 |
| ATOM | 338 | CB | PRO | 349 | 39.558 | 1.614 | 45.327 | 1.00 | 60.00 |
| ATOM | 339 | CG | PRO | 349 | 39.008 | 3.034 | 45.575 | 1.00 | 60.00 |
| ATOM | 340 | C | PRO | 349 | 41.486 | 0.350 | 46.425 | 1.00 | 60.00 |
| ATOM | 341 | O | PRO | 349 | 42.349 | 0.514 | 45.563 | 1.00 | 60.00 |
| ATOM | 342 | N | VAL | 350 | 41.442 | -0.704 | 47.259 | 1.00 | 60.00 |
| ATOM | 344 | CA | VAL | 350 | 42.426 | -1.737 | 47.213 | 1.00 | 60.00 |
| ATOM | 345 | CB | VAL | 350 | 43.285 | -1.798 | 48.441 | 1.00 | 60.00 |
| ATOM | 346 | CG1 | VAL | 350 | 42.379 | -2.090 | 49.649 | 1.00 | 60.00 |
| ATOM | 347 | CG2 | VAL | 350 | 44.379 | -2.856 | 48.224 | 1.00 | 60.00 |
| ATOM | 348 | C | VAL | 350 | 41.677 | -3.023 | 47.137 | 1.00 | 60.00 |
| ATOM | 349 | O | VAL | 350 | 40.582 | -3.149 | 47.684 | 1.00 | 60.00 |
| ATOM | 350 | N | ALA | 351 | 42.250 | -4.012 | 46.429 | 1.00 | 60.00 |
| ATOM | 352 | CA | ALA | 351 | 41.609 | -5.287 | 46.311 | 1.00 | 60.00 |
| ATOM | 353 | CB | ALA | 351 | 41.491 | -5.785 | 44.861 | 1.00 | 60.00 |
| ATOM | 354 | C | ALA | 351 | 42.473 | -6.255 | 47.046 | 1.00 | 60.00 |
| ATOM | 355 | O | ALA | 351 | 43.584 | -5.918 | 47.450 | 1.00 | 60.00 |
| ATOM | 356 | N | PHE | 352 | 41.974 | -7.487 | 47.264 | 1.00 | 60.00 |
| ATOM | 358 | CA | PHE | 352 | 42.778 | -8.437 | 47.974 | 1.00 | 60.00 |
| ATOM | 359 | CB | PHE | 352 | 42.087 | -9.007 | 49.226 | 1.00 | 60.00 |
| ATOM | 360 | CG | PHE | 352 | 43.030 | -9.963 | 49.871 | 1.00 | 60.00 |
| ATOM | 361 | CD1 | PHE | 352 | 44.096 | -9.492 | 50.603 | 1.00 | 60.00 |
| ATOM | 362 | CD2 | PHE | 352 | 42.811 | -11.320 | 49.813 | 1.00 | 60.00 |
| ATOM | 363 | CE1 | PHE | 352 | 44.955 | -10.359 | 51.235 | 1.00 | 60.00 |
| ATOM | 364 | CE2 | PHE | 352 | 43.661 | -12.192 | 50.452 | 1.00 | 60.00 |
| ATOM | 365 | CZ | PHE | 352 | 44.739 | -11.712 | 51.161 | 1.00 | 60.00 |
| ATOM | 366 | C | PHE | 352 | 43.092 | -9.582 | 47.065 | 1.00 | 60.00 |
| ATOM | 367 | O | PHE | 352 | 42.202 | -10.173 | 46.456 | 1.00 | 60.00 |
| ATOM | 368 | N | ARG | 353 | 44.394 | -9.908 | 46.946 | 1.00 | 60.00 |
| ATOM | 370 | CA | ARG | 353 | 44.828 | -10.999 | 46.123 | 1.00 | 60.00 |
| ATOM | 371 | CB | ARG | 353 | 44.901 | -10.663 | 44.623 | 1.00 | 60.00 |
| ATOM | 372 | CG | ARG | 353 | 43.555 | -10.313 | 43.988 | 1.00 | 60.00 |
| ATOM | 373 | CD | ARG | 353 | 43.617 | -10.218 | 42.462 | 1.00 | 60.00 |
| ATOM | 374 | NE | ARG | 353 | 44.677 | -9.228 | 42.122 | 1.00 | 60.00 |
| ATOM | 376 | CZ | ARG | 353 | 44.731 | -8.690 | 40.869 | 1.00 | 60.00 |
| ATOM | 377 | NH1 | ARG | 353 | 43.783 | -9.023 | 39.946 | 1.00 | 60.00 |
| ATOM | 380 | NH2 | ARG | 353 | 45.731 | -7.821 | 40.540 | 1.00 | 60.00 |
| ATOM | 383 | C | ARG | 353 | 46.228 | -11.284 | 46.553 | 1.00 | 60.00 |
| ATOM | 384 | O | ARG | 353 | 46.565 | -11.176 | 47.730 | 1.00 | 60.00 |
| ATOM | 385 | N | GLY | 354 | 47.083 | -11.675 | 45.590 | 1.00 | 60.00 |
| ATOM | 387 | CA | GLY | 354 | 48.461 | -11.908 | 45.900 | 1.00 | 60.00 |
| ATOM | 388 | C | GLY | 354 | 48.628 | -13.246 | 46.535 | 1.00 | 60.00 |
| ATOM | 389 | O | GLY | 354 | 49.468 | -13.421 | 47.417 | 1.00 | 60.00 |
| ATOM | 390 | N | ASP | 355 | 47.825 | -14.237 | 46.108 | 1.00 | 60.00 |
| ATOM | 392 | CA | ASP | 355 | 47.984 | -15.537 | 46.687 | 1.00 | 60.00 |
| ATOM | 393 | CB | ASP | 355 | 46.681 | -16.153 | 47.215 | 1.00 | 60.00 |
| ATOM | 394 | CG | ASP | 355 | 45.757 | -16.365 | 46.024 | 1.00 | 60.00 |
| ATOM | 395 | OD1 | ASP | 355 | 45.504 | -17.551 | 45.679 | 1.00 | 60.00 |
| ATOM | 396 | OD2 | ASP | 355 | 45.289 | -15.348 | 45.446 | 1.00 | 60.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 397 | C | ASP | 355 | 48.470 | -16.459 | 45.620 | 1.00 | 60.00 |
| ATOM | 398 | O | ASP | 355 | 48.219 | -16.249 | 44.435 | 1.00 | 60.00 |
| ATOM | 399 | N | SER | 356 | 49.208 | -17.508 | 46.031 | 1.00 | 60.00 |
| ATOM | 401 | CA | SER | 356 | 49.665 | -18.494 | 45.102 | 1.00 | 60.00 |
| ATOM | 402 | CB | SER | 356 | 51.181 | -18.759 | 45.157 | 1.00 | 60.00 |
| ATOM | 403 | OG | SER | 356 | 51.541 | -19.312 | 46.414 | 1.00 | 60.00 |
| ATOM | 405 | C | SER | 356 | 48.964 | -19.745 | 45.511 | 1.00 | 60.00 |
| ATOM | 406 | O | SER | 356 | 48.464 | -19.844 | 46.630 | 1.00 | 60.00 |
| ATOM | 407 | N | PHE | 357 | 48.891 | -20.736 | 44.605 | 1.00 | 60.00 |
| ATOM | 409 | CA | PHE | 357 | 48.189 | -21.935 | 44.948 | 1.00 | 60.00 |
| ATOM | 410 | CB | PHE | 357 | 47.958 | -22.864 | 43.742 | 1.00 | 60.00 |
| ATOM | 411 | CG | PHE | 357 | 47.190 | -24.055 | 44.203 | 1.00 | 60.00 |
| ATOM | 412 | CD1 | PHE | 357 | 47.831 | -25.123 | 44.790 | 1.00 | 60.00 |
| ATOM | 413 | CD2 | PHE | 357 | 45.832 | -24.125 | 43.999 | 1.00 | 60.00 |
| ATOM | 414 | CE1 | PHE | 357 | 47.123 | -26.237 | 45.175 | 1.00 | 60.00 |
| ATOM | 415 | CE2 | PHE | 357 | 45.118 | -25.238 | 44.379 | 1.00 | 60.00 |
| ATOM | 416 | CZ | PHE | 357 | 45.766 | -26.298 | 44.967 | 1.00 | 60.00 |
| ATOM | 417 | C | PHE | 357 | 49.029 | -22.664 | 45.942 | 1.00 | 60.00 |
| ATOM | 418 | O | PHE | 357 | 50.005 | -23.320 | 45.583 | 1.00 | 60.00 |
| ATOM | 419 | N | THR | 358 | 48.674 | -22.547 | 47.236 | 1.00 | 60.00 |
| ATOM | 421 | CA | THR | 358 | 49.444 | -23.220 | 48.238 | 1.00 | 60.00 |
| ATOM | 422 | CB | THR | 358 | 50.377 | -22.305 | 48.975 | 1.00 | 60.00 |
| ATOM | 423 | OG1 | THR | 358 | 51.242 | -23.055 | 49.814 | 1.00 | 60.00 |
| ATOM | 425 | CG2 | THR | 358 | 49.546 | -21.314 | 49.809 | 1.00 | 60.00 |
| ATOM | 426 | C | THR | 358 | 48.515 | -23.828 | 49.240 | 1.00 | 60.00 |
| ATOM | 427 | O | THR | 358 | 47.512 | -23.229 | 49.627 | 1.00 | 60.00 |
| ATOM | 428 | N | HIS | 359 | 48.825 | -25.068 | 49.661 | 1.00 | 60.00 |
| ATOM | 430 | CA | HIS | 359 | 48.031 | -25.756 | 50.636 | 1.00 | 60.00 |
| ATOM | 431 | CB | HIS | 359 | 48.406 | -27.241 | 50.750 | 1.00 | 60.00 |
| ATOM | 432 | CG | HIS | 359 | 48.261 | -27.982 | 49.456 | 1.00 | 60.00 |
| ATOM | 433 | CD2 | HIS | 359 | 47.273 | -28.810 | 49.019 | 1.00 | 60.00 |
| ATOM | 434 | ND1 | HIS | 359 | 49.184 | -27.927 | 48.435 | 1.00 | 60.00 |
| ATOM | 436 | CE1 | HIS | 359 | 48.713 | -28.717 | 47.439 | 1.00 | 60.00 |
| ATOM | 437 | NE2 | HIS | 359 | 47.556 | -29.275 | 47.747 | 1.00 | 60.00 |
| ATOM | 439 | C | HIS | 359 | 48.286 | -25.152 | 51.980 | 1.00 | 60.00 |
| ATOM | 440 | O | HIS | 359 | 47.362 | -24.901 | 52.753 | 1.00 | 60.00 |
| ATOM | 441 | N | THR | 360 | 49.573 | -24.886 | 52.275 | 1.00 | 60.00 |
| ATOM | 443 | CA | THR | 360 | 49.971 | -24.398 | 53.563 | 1.00 | 60.00 |
| ATOM | 444 | CB | THR | 360 | 51.419 | -24.013 | 53.638 | 1.00 | 60.00 |
| ATOM | 445 | OG1 | THR | 360 | 51.804 | -23.813 | 54.990 | 1.00 | 60.00 |
| ATOM | 447 | CG2 | THR | 360 | 51.624 | -22.718 | 52.833 | 1.00 | 60.00 |
| ATOM | 448 | C | THR | 360 | 49.166 | -23.203 | 53.939 | 1.00 | 60.00 |
| ATOM | 449 | O | THR | 360 | 48.683 | -22.445 | 53.098 | 1.00 | 60.00 |
| ATOM | 450 | N | PRO | 361 | 48.991 | -23.059 | 55.221 | 1.00 | 60.00 |
| ATOM | 451 | CD | PRO | 361 | 48.870 | -24.216 | 56.090 | 1.00 | 60.00 |
| ATOM | 452 | CA | PRO | 361 | 48.265 | -21.932 | 55.724 | 1.00 | 60.00 |
| ATOM | 453 | CB | PRO | 361 | 47.721 | -22.343 | 57.095 | 1.00 | 60.00 |
| ATOM | 454 | CG | PRO | 361 | 48.502 | -23.620 | 57.456 | 1.00 | 60.00 |
| ATOM | 455 | C | PRO | 361 | 49.167 | -20.745 | 55.759 | 1.00 | 60.00 |
| ATOM | 456 | O | PRO | 361 | 50.356 | -20.899 | 56.035 | 1.00 | 60.00 |
| ATOM | 457 | N | PRO | 362 | 48.624 | -19.595 | 55.497 | 1.00 | 60.00 |
| ATOM | 458 | CD | PRO | 362 | 47.213 | -19.348 | 55.739 | 1.00 | 60.00 |
| ATOM | 459 | CA | PRO | 362 | 49.387 | -18.382 | 55.475 | 1.00 | 60.00 |
| ATOM | 460 | CB | PRO | 362 | 48.366 | -17.271 | 55.254 | 1.00 | 60.00 |
| ATOM | 461 | CG | PRO | 362 | 47.104 | -17.827 | 55.939 | 1.00 | 60.00 |
| ATOM | 462 | C | PRO | 362 | 50.049 | -18.232 | 56.803 | 1.00 | 60.00 |
| ATOM | 463 | O | PRO | 362 | 49.509 | -18.719 | 57.795 | 1.00 | 60.00 |
| ATOM | 464 | N | LEU | 363 | 51.229 | -17.585 | 56.840 | 1.00 | 60.00 |
| ATOM | 466 | CA | LEU | 363 | 51.885 | -17.368 | 58.091 | 1.00 | 60.00 |
| ATOM | 467 | CB | LEU | 363 | 53.225 | -16.627 | 57.946 | 1.00 | 60.00 |
| ATOM | 468 | CG | LEU | 363 | 53.937 | -16.380 | 59.289 | 1.00 | 60.00 |
| ATOM | 469 | CD1 | LEU | 363 | 54.300 | -17.700 | 59.983 | 1.00 | 60.00 |
| ATOM | 470 | CD2 | LEU | 363 | 55.146 | -15.448 | 59.115 | 1.00 | 60.00 |
| ATOM | 471 | C | LEU | 363 | 50.973 | -16.498 | 58.880 | 1.00 | 60.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 472 | O | LEU | 363 | 50.651 | -16.791 | 60.030 | 1.00 | 60.00 |
| ATOM | 473 | N | ASP | 364 | 50.514 | -15.401 | 58.255 | 1.00 | 60.00 |
| ATOM | 475 | CA | ASP | 364 | 49.614 | -14.521 | 58.928 | 1.00 | 60.00 |
| ATOM | 476 | CB | ASP | 364 | 49.691 | -13.063 | 58.441 | 1.00 | 60.00 |
| ATOM | 477 | CG | ASP | 364 | 51.035 | -12.490 | 58.861 | 1.00 | 60.00 |
| ATOM | 478 | OD1 | ASP | 364 | 51.297 | -11.302 | 58.532 | 1.00 | 60.00 |
| ATOM | 479 | OD2 | ASP | 364 | 51.820 | -13.232 | 59.511 | 1.00 | 60.00 |
| ATOM | 480 | C | ASP | 364 | 48.249 | -15.013 | 58.601 | 1.00 | 60.00 |
| ATOM | 481 | O | ASP | 364 | 48.075 | -16.007 | 57.898 | 1.00 | 60.00 |
| ATOM | 482 | N | PRO | 365 | 47.273 | -14.343 | 59.135 | 1.00 | 60.00 |
| ATOM | 483 | CD | PRO | 365 | 47.390 | -13.790 | 60.473 | 1.00 | 60.00 |
| ATOM | 484 | CA | PRO | 365 | 45.920 | -14.690 | 58.816 | 1.00 | 60.00 |
| ATOM | 485 | CB | PRO | 365 | 45.060 | -14.202 | 59.985 | 1.00 | 60.00 |
| ATOM | 486 | CG | PRO | 365 | 45.982 | -13.264 | 60.784 | 1.00 | 60.00 |
| ATOM | 487 | C | PRO | 365 | 45.602 | -14.043 | 57.512 | 1.00 | 60.00 |
| ATOM | 488 | O | PRO | 365 | 46.289 | -13.094 | 57.136 | 1.00 | 60.00 |
| ATOM | 489 | N | GLN | 366 | 44.578 | -14.538 | 56.796 | 1.00 | 60.00 |
| ATOM | 491 | CA | GLN | 366 | 44.261 | -13.941 | 55.537 | 1.00 | 60.00 |
| ATOM | 492 | CB | GLN | 366 | 43.136 | -14.680 | 54.789 | 1.00 | 60.00 |
| ATOM | 493 | CG | GLN | 366 | 43.557 | -16.094 | 54.371 | 1.00 | 60.00 |
| ATOM | 494 | CD | GLN | 366 | 42.408 | -16.769 | 53.636 | 1.00 | 60.00 |
| ATOM | 495 | OE1 | GLN | 366 | 42.506 | -17.940 | 53.271 | 1.00 | 60.00 |
| ATOM | 496 | NE2 | GLN | 366 | 41.297 | -16.021 | 53.404 | 1.00 | 60.00 |
| ATOM | 499 | C | GLN | 366 | 43.854 | -12.534 | 55.822 | 1.00 | 60.00 |
| ATOM | 500 | O | GLN | 366 | 44.212 | -11.612 | 55.090 | 1.00 | 60.00 |
| ATOM | 501 | N | GLU | 367 | 43.102 | -12.332 | 56.920 | 1.00 | 60.00 |
| ATOM | 503 | CA | GLU | 367 | 42.701 | -11.010 | 57.300 | 1.00 | 60.00 |
| ATOM | 504 | CB | GLU | 367 | 41.684 | -11.013 | 58.454 | 1.00 | 60.00 |
| ATOM | 505 | CG | GLU | 367 | 42.187 | -11.759 | 59.692 | 1.00 | 60.00 |
| ATOM | 506 | CD | GLU | 367 | 41.045 | -11.857 | 60.693 | 1.00 | 60.00 |
| ATOM | 507 | OE1 | GLU | 367 | 40.612 | -10.795 | 61.212 | 1.00 | 60.00 |
| ATOM | 508 | OE2 | GLU | 367 | 40.589 | -13.004 | 60.951 | 1.00 | 60.00 |
| ATOM | 509 | C | GLU | 367 | 43.940 | -10.300 | 57.747 | 1.00 | 60.00 |
| ATOM | 510 | O | GLU | 367 | 44.893 | -10.933 | 58.198 | 1.00 | 60.00 |
| ATOM | 511 | N | LEU | 368 | 43.971 | -8.958 | 57.610 | 1.00 | 40.00 |
| ATOM | 513 | CA | LEU | 368 | 45.148 | -8.233 | 57.992 | 1.00 | 40.00 |
| ATOM | 514 | CB | LEU | 368 | 45.817 | -7.526 | 56.792 | 1.00 | 40.00 |
| ATOM | 515 | CG | LEU | 368 | 47.098 | -6.716 | 57.097 | 1.00 | 40.00 |
| ATOM | 516 | CD1 | LEU | 368 | 46.823 | -5.435 | 57.902 | 1.00 | 40.00 |
| ATOM | 517 | CD2 | LEU | 368 | 48.171 | -7.612 | 57.734 | 1.00 | 40.00 |
| ATOM | 518 | C | LEU | 368 | 44.735 | -7.199 | 58.981 | 1.00 | 40.00 |
| ATOM | 519 | O | LEU | 368 | 43.798 | -6.437 | 58.752 | 1.00 | 40.00 |
| ATOM | 520 | N | ASP | 369 | 45.427 | -7.161 | 60.132 | 1.00 | 40.00 |
| ATOM | 522 | CA | ASP | 369 | 45.144 | -6.135 | 61.082 | 1.00 | 40.00 |
| ATOM | 523 | CB | ASP | 369 | 45.333 | -6.552 | 62.551 | 1.00 | 40.00 |
| ATOM | 524 | CG | ASP | 369 | 44.269 | -7.568 | 62.932 | 1.00 | 40.00 |
| ATOM | 525 | OD1 | ASP | 369 | 44.164 | -7.875 | 64.150 | 1.00 | 40.00 |
| ATOM | 526 | OD2 | ASP | 369 | 43.553 | -8.056 | 62.018 | 1.00 | 40.00 |
| ATOM | 527 | C | ASP | 369 | 46.245 | -5.196 | 60.786 | 1.00 | 40.00 |
| ATOM | 528 | O | ASP | 369 | 47.393 | -5.629 | 60.696 | 1.00 | 40.00 |
| ATOM | 529 | N | ILE | 370 | 45.918 | -3.906 | 60.581 | 1.00 | 40.00 |
| ATOM | 531 | CA | ILE | 370 | 46.965 | -2.968 | 60.332 | 1.00 | 40.00 |
| ATOM | 532 | CB | ILE | 370 | 46.459 | -1.569 | 60.186 | 1.00 | 40.00 |
| ATOM | 533 | CG2 | ILE | 370 | 47.655 | -0.605 | 60.196 | 1.00 | 40.00 |
| ATOM | 534 | CG1 | ILE | 370 | 45.594 | -1.485 | 58.919 | 1.00 | 40.00 |
| ATOM | 535 | CD1 | ILE | 370 | 44.814 | -0.183 | 58.792 | 1.00 | 40.00 |
| ATOM | 536 | C | ILE | 370 | 47.813 | -3.082 | 61.542 | 1.00 | 40.00 |
| ATOM | 537 | O | ILE | 370 | 48.973 | -3.478 | 61.441 | 1.00 | 40.00 |
| ATOM | 538 | N | LEU | 371 | 47.230 | -2.776 | 62.718 | 1.00 | 40.00 |
| ATOM | 540 | CA | LEU | 371 | 47.927 | -3.049 | 63.936 | 1.00 | 40.00 |
| ATOM | 541 | CB | LEU | 371 | 49.402 | -2.609 | 63.988 | 1.00 | 40.00 |
| ATOM | 542 | CG | LEU | 371 | 50.110 | -3.093 | 65.267 | 1.00 | 40.00 |
| ATOM | 543 | CD1 | LEU | 371 | 50.003 | -4.621 | 65.407 | 1.00 | 40.00 |
| ATOM | 544 | CD2 | LEU | 371 | 51.575 | -2.632 | 65.301 | 1.00 | 40.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 545 | C | LEU | 371 | 47.234 | -2.413 | 65.087 | 1.00 | 40.00 |
| ATOM | 546 | O | LEU | 371 | 46.575 | -1.382 | 64.958 | 1.00 | 40.00 |
| ATOM | 547 | N | LYS | 372 | 47.392 | -3.051 | 66.257 | 1.00 | 20.00 |
| ATOM | 549 | CA | LYS | 372 | 46.865 | -2.593 | 67.503 | 1.00 | 20.00 |
| ATOM | 550 | CB | LYS | 372 | 47.005 | -3.637 | 68.625 | 1.00 | 20.00 |
| ATOM | 551 | CG | LYS | 372 | 46.173 | -4.896 | 68.358 | 1.00 | 20.00 |
| ATOM | 552 | CD | LYS | 372 | 46.478 | -6.068 | 69.293 | 1.00 | 20.00 |
| ATOM | 553 | CE | LYS | 372 | 45.536 | -6.144 | 70.496 | 1.00 | 20.00 |
| ATOM | 554 | NZ | LYS | 372 | 45.826 | -7.358 | 71.292 | 1.00 | 20.00 |
| ATOM | 558 | C | LYS | 372 | 47.650 | -1.374 | 67.857 | 1.00 | 20.00 |
| ATOM | 559 | O | LYS | 372 | 47.230 | -0.550 | 68.665 | 1.00 | 20.00 |
| ATOM | 560 | N | THR | 373 | 48.841 | -1.234 | 67.255 | 1.00 | 20.00 |
| ATOM | 562 | CA | THR | 373 | 49.713 | -0.143 | 67.570 | 1.00 | 20.00 |
| ATOM | 563 | CB | THR | 373 | 50.993 | -0.161 | 66.790 | 1.00 | 20.00 |
| ATOM | 564 | OG1 | THR | 373 | 51.913 | 0.773 | 67.334 | 1.00 | 20.00 |
| ATOM | 566 | CG2 | THR | 373 | 50.677 | 0.195 | 65.327 | 1.00 | 20.00 |
| ATOM | 567 | C | THR | 373 | 49.078 | 1.188 | 67.308 | 1.00 | 20.00 |
| ATOM | 568 | O | THR | 373 | 49.377 | 2.153 | 68.009 | 1.00 | 20.00 |
| ATOM | 569 | N | VAL | 374 | 48.194 | 1.295 | 66.295 | 1.00 | 20.00 |
| ATOM | 571 | CA | VAL | 374 | 47.677 | 2.593 | 65.946 | 1.00 | 20.00 |
| ATOM | 572 | CB | VAL | 374 | 47.137 | 2.637 | 64.544 | 1.00 | 20.00 |
| ATOM | 573 | CG1 | VAL | 374 | 46.601 | 4.051 | 64.263 | 1.00 | 20.00 |
| ATOM | 574 | CG2 | VAL | 374 | 48.245 | 2.177 | 63.578 | 1.00 | 20.00 |
| ATOM | 575 | C | VAL | 374 | 46.591 | 3.087 | 66.859 | 1.00 | 20.00 |
| ATOM | 576 | O | VAL | 374 | 45.431 | 2.689 | 66.736 | 1.00 | 20.00 |
| ATOM | 577 | N | LYS | 375 | 46.980 | 3.924 | 67.848 | 1.00 | 20.00 |
| ATOM | 579 | CA | LYS | 375 | 46.084 | 4.602 | 68.746 | 1.00 | 20.00 |
| ATOM | 580 | CB | LYS | 375 | 46.752 | 5.075 | 70.049 | 1.00 | 20.00 |
| ATOM | 581 | CG | LYS | 375 | 47.091 | 3.970 | 71.050 | 1.00 | 20.00 |
| ATOM | 582 | CD | LYS | 375 | 47.814 | 4.503 | 72.289 | 1.00 | 20.00 |
| ATOM | 583 | CE | LYS | 375 | 47.964 | 3.476 | 73.413 | 1.00 | 20.00 |
| ATOM | 584 | NZ | LYS | 375 | 48.533 | 4.126 | 74.615 | 1.00 | 20.00 |
| ATOM | 588 | C | LYS | 375 | 45.439 | 5.830 | 68.169 | 1.00 | 20.00 |
| ATOM | 589 | O | LYS | 375 | 44.256 | 6.079 | 68.386 | 1.00 | 20.00 |
| ATOM | 590 | N | GLU | 376 | 46.193 | 6.658 | 67.419 | 1.00 | 20.00 |
| ATOM | 592 | CA | GLU | 376 | 45.613 | 7.918 | 67.049 | 1.00 | 20.00 |
| ATOM | 593 | CB | GLU | 376 | 46.103 | 9.051 | 67.971 | 1.00 | 20.00 |
| ATOM | 594 | CG | GLU | 376 | 45.540 | 10.438 | 67.665 | 1.00 | 20.00 |
| ATOM | 595 | CD | GLU | 376 | 46.126 | 11.397 | 68.691 | 1.00 | 20.00 |
| ATOM | 596 | OE1 | GLU | 376 | 45.997 | 11.108 | 69.911 | 1.00 | 20.00 |
| ATOM | 597 | OE2 | GLU | 376 | 46.716 | 12.426 | 68.269 | 1.00 | 20.00 |
| ATOM | 598 | C | GLU | 376 | 45.926 | 8.309 | 65.641 | 1.00 | 20.00 |
| ATOM | 599 | O | GLU | 376 | 46.796 | 7.732 | 64.994 | 1.00 | 20.00 |
| ATOM | 600 | N | ILE | 377 | 45.148 | 9.283 | 65.121 | 1.00 | 20.00 |
| ATOM | 602 | CA | ILE | 377 | 45.362 | 9.865 | 63.833 | 1.00 | 20.00 |
| ATOM | 603 | CB | ILE | 377 | 44.403 | 9.370 | 62.791 | 1.00 | 20.00 |
| ATOM | 604 | CG2 | ILE | 377 | 44.680 | 10.133 | 61.485 | 1.00 | 20.00 |
| ATOM | 605 | CG1 | ILE | 377 | 44.526 | 7.844 | 62.642 | 1.00 | 20.00 |
| ATOM | 606 | CD1 | ILE | 377 | 43.402 | 7.214 | 61.820 | 1.00 | 20.00 |
| ATOM | 607 | C | ILE | 377 | 45.075 | 11.311 | 64.089 | 1.00 | 20.00 |
| ATOM | 608 | O | ILE | 377 | 44.015 | 11.662 | 64.599 | 1.00 | 20.00 |
| ATOM | 609 | N | THR | 378 | 46.029 | 12.183 | 63.740 | 1.00 | 20.00 |
| ATOM | 611 | CA | THR | 378 | 45.985 | 13.594 | 63.994 | 1.00 | 20.00 |
| ATOM | 612 | CB | THR | 378 | 47.317 | 14.235 | 63.734 | 1.00 | 20.00 |
| ATOM | 613 | OG1 | THR | 378 | 48.316 | 13.599 | 64.516 | 1.00 | 20.00 |
| ATOM | 615 | CG2 | THR | 378 | 47.249 | 15.718 | 64.124 | 1.00 | 20.00 |
| ATOM | 616 | C | THR | 378 | 44.965 | 14.303 | 63.159 | 1.00 | 20.00 |
| ATOM | 617 | O | THR | 378 | 44.612 | 15.442 | 63.452 | 1.00 | 20.00 |
| ATOM | 618 | N | GLY | 379 | 44.522 | 13.695 | 62.044 | 1.00 | 20.00 |
| ATOM | 620 | CA | GLY | 379 | 43.608 | 14.380 | 61.171 | 1.00 | 20.00 |
| ATOM | 621 | C | GLY | 379 | 42.325 | 13.631 | 61.001 | 1.00 | 20.00 |
| ATOM | 622 | O | GLY | 379 | 41.520 | 13.523 | 61.923 | 1.00 | 20.00 |
| ATOM | 623 | N | PHE | 380 | 42.082 | 13.126 | 59.775 | 1.00 | 20.00 |
| ATOM | 625 | CA | PHE | 380 | 40.869 | 12.405 | 59.515 | 1.00 | 20.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 626 | CB | PHE | 380 | 39.920 | 13.116 | 58.530 | 1.00 | 20.00 |
| ATOM | 627 | CG | PHE | 380 | 40.598 | 13.264 | 57.212 | 1.00 | 20.00 |
| ATOM | 628 | CD1 | PHE | 380 | 40.528 | 12.265 | 56.268 | 1.00 | 20.00 |
| ATOM | 629 | CD2 | PHE | 380 | 41.265 | 14.427 | 56.902 | 1.00 | 20.00 |
| ATOM | 630 | CE1 | PHE | 380 | 41.112 | 12.426 | 55.034 | 1.00 | 20.00 |
| ATOM | 631 | CE2 | PHE | 380 | 41.860 | 14.590 | 55.674 | 1.00 | 20.00 |
| ATOM | 632 | CZ | PHE | 380 | 41.780 | 13.589 | 54.736 | 1.00 | 20.00 |
| ATOM | 633 | C | PHE | 380 | 41.216 | 11.066 | 58.955 | 1.00 | 20.00 |
| ATOM | 634 | O | PHE | 380 | 42.359 | 10.824 | 58.573 | 1.00 | 20.00 |
| ATOM | 635 | N | LEU | 381 | 40.231 | 10.141 | 58.942 | 1.00 | 20.00 |
| ATOM | 637 | CA | LEU | 381 | 40.454 | 8.822 | 58.422 | 1.00 | 20.00 |
| ATOM | 638 | CB | LEU | 381 | 40.156 | 7.725 | 59.462 | 1.00 | 20.00 |
| ATOM | 639 | CG | LEU | 381 | 40.369 | 6.281 | 58.972 | 1.00 | 20.00 |
| ATOM | 640 | CD1 | LEU | 381 | 41.834 | 6.032 | 58.580 | 1.00 | 20.00 |
| ATOM | 641 | CD2 | LEU | 381 | 39.866 | 5.268 | 60.015 | 1.00 | 20.00 |
| ATOM | 642 | C | LEU | 381 | 39.534 | 8.629 | 57.251 | 1.00 | 20.00 |
| ATOM | 643 | O | LEU | 381 | 38.318 | 8.782 | 57.368 | 1.00 | 20.00 |
| ATOM | 644 | N | LEU | 382 | 40.096 | 8.290 | 56.073 | 1.00 | 20.00 |
| ATOM | 646 | CA | LEU | 382 | 39.283 | 8.132 | 54.899 | 1.00 | 20.00 |
| ATOM | 647 | CB | LEU | 382 | 39.642 | 9.158 | 53.808 | 1.00 | 20.00 |
| ATOM | 648 | CG | LEU | 382 | 38.818 | 9.062 | 52.511 | 1.00 | 20.00 |
| ATOM | 649 | CD1 | LEU | 382 | 37.330 | 9.337 | 52.761 | 1.00 | 20.00 |
| ATOM | 650 | CD2 | LEU | 382 | 39.405 | 9.975 | 51.424 | 1.00 | 20.00 |
| ATOM | 651 | C | LEU | 382 | 39.459 | 6.767 | 54.312 | 1.00 | 20.00 |
| ATOM | 652 | O | LEU | 382 | 40.548 | 6.399 | 53.873 | 1.00 | 20.00 |
| ATOM | 653 | N | ILE | 383 | 38.375 | 5.968 | 54.295 | 1.00 | 20.00 |
| ATOM | 655 | CA | ILE | 383 | 38.451 | 4.677 | 53.681 | 1.00 | 20.00 |
| ATOM | 656 | CB | ILE | 383 | 38.143 | 3.540 | 54.623 | 1.00 | 20.00 |
| ATOM | 657 | CG2 | ILE | 383 | 36.747 | 3.739 | 55.239 | 1.00 | 20.00 |
| ATOM | 658 | CG1 | ILE | 383 | 38.351 | 2.191 | 53.916 | 1.00 | 20.00 |
| ATOM | 659 | CD1 | ILE | 383 | 38.352 | 1.000 | 54.872 | 1.00 | 20.00 |
| ATOM | 660 | C | ILE | 383 | 37.471 | 4.676 | 52.553 | 1.00 | 20.00 |
| ATOM | 661 | O | ILE | 383 | 36.259 | 4.747 | 52.745 | 1.00 | 20.00 |
| ATOM | 662 | N | GLN | 384 | 37.975 | 4.608 | 51.314 | 1.00 | 20.00 |
| ATOM | 664 | CA | GLN | 384 | 37.065 | 4.622 | 50.213 | 1.00 | 20.00 |
| ATOM | 665 | CB | GLN | 384 | 37.334 | 5.758 | 49.212 | 1.00 | 20.00 |
| ATOM | 666 | CG | GLN | 384 | 36.365 | 5.786 | 48.026 | 1.00 | 20.00 |
| ATOM | 667 | CD | GLN | 384 | 36.804 | 6.908 | 47.092 | 1.00 | 20.00 |
| ATOM | 668 | OE1 | GLN | 384 | 37.864 | 7.503 | 47.279 | 1.00 | 20.00 |
| ATOM | 669 | NE2 | GLN | 384 | 35.972 | 7.208 | 46.058 | 1.00 | 20.00 |
| ATOM | 672 | C | GLN | 384 | 37.241 | 3.340 | 49.472 | 1.00 | 20.00 |
| ATOM | 673 | O | GLN | 384 | 38.359 | 2.852 | 49.313 | 1.00 | 20.00 |
| ATOM | 674 | N | ALA | 385 | 36.108 | 2.768 | 49.020 | 1.00 | 20.00 |
| ATOM | 676 | CA | ALA | 385 | 36.047 | 1.565 | 48.240 | 1.00 | 20.00 |
| ATOM | 677 | CB | ALA | 385 | 36.094 | 1.823 | 46.723 | 1.00 | 20.00 |
| ATOM | 678 | C | ALA | 385 | 37.093 | 0.547 | 48.564 | 1.00 | 20.00 |
| ATOM | 679 | O | ALA | 385 | 38.095 | 0.433 | 47.860 | 1.00 | 20.00 |
| ATOM | 680 | N | TRP | 386 | 36.905 | -0.206 | 49.665 | 1.00 | 40.00 |
| ATOM | 682 | CA | TRP | 386 | 37.807 | -1.282 | 49.951 | 1.00 | 40.00 |
| ATOM | 683 | CB | TRP | 386 | 38.698 | -1.047 | 51.187 | 1.00 | 40.00 |
| ATOM | 684 | CG | TRP | 386 | 39.643 | -2.188 | 51.498 | 1.00 | 40.00 |
| ATOM | 685 | CD2 | TRP | 386 | 40.808 | -2.083 | 52.333 | 1.00 | 40.00 |
| ATOM | 686 | CE2 | TRP | 386 | 41.411 | -3.341 | 52.364 | 1.00 | 40.00 |
| ATOM | 687 | CE3 | TRP | 386 | 41.335 | -1.026 | 53.017 | 1.00 | 40.00 |
| ATOM | 688 | CD1 | TRP | 386 | 39.602 | -3.478 | 51.060 | 1.00 | 40.00 |
| ATOM | 689 | NE1 | TRP | 386 | 40.658 | -4.188 | 51.581 | 1.00 | 40.00 |
| ATOM | 691 | CZ2 | TRP | 386 | 42.553 | -3.560 | 53.080 | 1.00 | 40.00 |
| ATOM | 692 | CZ3 | TRP | 386 | 42.485 | -1.251 | 53.740 | 1.00 | 40.00 |
| ATOM | 693 | CH2 | TRP | 386 | 43.085 | -2.492 | 53.768 | 1.00 | 40.00 |
| ATOM | 694 | C | TRP | 386 | 36.955 | -2.481 | 50.219 | 1.00 | 40.00 |
| ATOM | 695 | O | TRP | 386 | 36.205 | -2.513 | 51.194 | 1.00 | 40.00 |
| ATOM | 696 | N | PRO | 387 | 37.010 | -3.458 | 49.359 | 1.00 | 40.00 |
| ATOM | 697 | CD | PRO | 387 | 37.070 | -3.165 | 47.936 | 1.00 | 40.00 |
| ATOM | 698 | CA | PRO | 387 | 36.218 | -4.629 | 49.623 | 1.00 | 40.00 |

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|------|-----|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 699 | CB | PRO | 387 | 35.733 | -5.146 | 48.267 | 1.00 | 40.00 |
| ATOM | 700 | CG | PRO | 387 | 36.669 | -4.479 | 47.248 | 1.00 | 40.00 |
| ATOM | 701 | C | PRO | 387 | 36.983 | -5.651 | 50.398 | 1.00 | 40.00 |
| ATOM | 702 | O | PRO | 387 | 38.205 | -5.705 | 50.273 | 1.00 | 40.00 |
| ATOM | 703 | N | GLU | 388 | 36.281 | -6.468 | 51.211 | 1.00 | 60.00 |
| ATOM | 705 | CA | GLU | 388 | 36.926 | -7.544 | 51.902 | 1.00 | 60.00 |
| ATOM | 706 | CB | GLU | 388 | 38.009 | -7.126 | 52.913 | 1.00 | 60.00 |
| ATOM | 707 | CG | GLU | 388 | 37.503 | -6.355 | 54.129 | 1.00 | 60.00 |
| ATOM | 708 | CD | GLU | 388 | 38.681 | -6.251 | 55.088 | 1.00 | 60.00 |
| ATOM | 709 | OE1 | GLU | 388 | 38.438 | -6.226 | 56.323 | 1.00 | 60.00 |
| ATOM | 710 | OE2 | GLU | 388 | 39.841 | -6.199 | 54.597 | 1.00 | 60.00 |
| ATOM | 711 | C | GLU | 388 | 35.886 | -8.334 | 52.631 | 1.00 | 60.00 |
| ATOM | 712 | O | GLU | 388 | 34.735 | -7.917 | 52.752 | 1.00 | 60.00 |
| ATOM | 713 | N | ASN | 389 | 36.284 | -9.524 | 53.118 | 1.00 | 60.00 |
| ATOM | 715 | CA | ASN | 389 | 35.397 | -10.427 | 53.793 | 1.00 | 60.00 |
| ATOM | 716 | CB | ASN | 389 | 36.064 | -11.789 | 54.065 | 1.00 | 60.00 |
| ATOM | 717 | CG | ASN | 389 | 35.053 | -12.711 | 54.733 | 1.00 | 60.00 |
| ATOM | 718 | OD1 | ASN | 389 | 33.860 | -12.668 | 54.438 | 1.00 | 60.00 |
| ATOM | 719 | ND2 | ASN | 389 | 35.546 | -13.572 | 55.664 | 1.00 | 60.00 |
| ATOM | 722 | C | ASN | 389 | 34.935 | -9.900 | 55.114 | 1.00 | 60.00 |
| ATOM | 723 | O | ASN | 389 | 33.736 | -9.844 | 55.382 | 1.00 | 60.00 |
| ATOM | 724 | N | ARG | 390 | 35.880 | -9.474 | 55.972 | 1.00 | 60.00 |
| ATOM | 726 | CA | ARG | 390 | 35.501 | -9.094 | 57.300 | 1.00 | 60.00 |
| ATOM | 727 | CB | ARG | 390 | 36.509 | -9.551 | 58.362 | 1.00 | 60.00 |
| ATOM | 728 | CG | ARG | 390 | 36.820 | -11.045 | 58.294 | 1.00 | 60.00 |
| ATOM | 729 | CD | ARG | 390 | 37.813 | -11.498 | 59.364 | 1.00 | 60.00 |
| ATOM | 730 | NE | ARG | 390 | 38.361 | -12.814 | 58.936 | 1.00 | 60.00 |
| ATOM | 732 | CZ | ARG | 390 | 37.702 | -13.969 | 59.241 | 1.00 | 60.00 |
| ATOM | 733 | NH1 | ARG | 390 | 38.230 | -15.169 | 58.863 | 1.00 | 60.00 |
| ATOM | 736 | NH2 | ARG | 390 | 36.522 | -13.923 | 59.925 | 1.00 | 60.00 |
| ATOM | 739 | C | ARG | 390 | 35.418 | -7.612 | 57.417 | 1.00 | 60.00 |
| ATOM | 740 | O | ARG | 390 | 35.440 | -6.887 | 56.423 | 1.00 | 60.00 |
| ATOM | 741 | N | THR | 391 | 35.301 | -7.131 | 58.670 | 1.00 | 60.00 |
| ATOM | 743 | CA | THR | 391 | 35.236 | -5.722 | 58.895 | 1.00 | 60.00 |
| ATOM | 744 | CB | THR | 391 | 34.997 | -5.337 | 60.326 | 1.00 | 60.00 |
| ATOM | 745 | OG1 | THR | 391 | 36.067 | -5.792 | 61.141 | 1.00 | 60.00 |
| ATOM | 747 | CG2 | THR | 391 | 33.669 | -5.954 | 60.793 | 1.00 | 60.00 |
| ATOM | 748 | C | THR | 391 | 36.572 | -5.192 | 58.519 | 1.00 | 60.00 |
| ATOM | 749 | O | THR | 391 | 37.595 | -5.622 | 59.045 | 1.00 | 60.00 |
| ATOM | 750 | N | ASP | 392 | 36.586 | -4.236 | 57.579 | 1.00 | 60.00 |
| ATOM | 752 | CA | ASP | 392 | 37.814 | -3.675 | 57.114 | 1.00 | 60.00 |
| ATOM | 753 | CB | ASP | 392 | 37.609 | -2.694 | 55.949 | 1.00 | 60.00 |
| ATOM | 754 | CG | ASP | 392 | 38.951 | -2.481 | 55.266 | 1.00 | 60.00 |
| ATOM | 755 | OD1 | ASP | 392 | 39.929 | -3.181 | 55.641 | 1.00 | 60.00 |
| ATOM | 756 | OD2 | ASP | 392 | 39.012 | -1.613 | 54.355 | 1.00 | 60.00 |
| ATOM | 757 | C | ASP | 392 | 38.410 | -2.927 | 58.259 | 1.00 | 60.00 |
| ATOM | 758 | O | ASP | 392 | 39.629 | -2.870 | 58.415 | 1.00 | 60.00 |
| ATOM | 759 | N | LEU | 393 | 37.542 | -2.351 | 59.111 | 1.00 | 40.00 |
| ATOM | 761 | CA | LEU | 393 | 37.993 | -1.561 | 60.212 | 1.00 | 40.00 |
| ATOM | 762 | CB | LEU | 393 | 36.881 | -0.757 | 60.882 | 1.00 | 40.00 |
| ATOM | 763 | CG | LEU | 393 | 36.203 | 0.250 | 59.929 | 1.00 | 40.00 |
| ATOM | 764 | CD1 | LEU | 393 | 37.198 | 1.308 | 59.425 | 1.00 | 40.00 |
| ATOM | 765 | CD2 | LEU | 393 | 35.465 | -0.465 | 58.787 | 1.00 | 40.00 |
| ATOM | 766 | C | LEU | 393 | 38.699 | -2.424 | 61.212 | 1.00 | 40.00 |
| ATOM | 767 | O | LEU | 393 | 39.431 | -1.924 | 62.064 | 1.00 | 40.00 |
| ATOM | 768 | N | HIS | 394 | 38.494 | -3.755 | 61.128 | 1.00 | 40.00 |
| ATOM | 770 | CA | HIS | 394 | 39.064 | -4.696 | 62.056 | 1.00 | 40.00 |
| ATOM | 771 | CB | HIS | 394 | 38.835 | -6.171 | 61.670 | 1.00 | 40.00 |
| ATOM | 772 | CG | HIS | 394 | 39.918 | -6.759 | 60.813 | 1.00 | 40.00 |
| ATOM | 773 | CD2 | HIS | 394 | 40.944 | -7.577 | 61.173 | 1.00 | 40.00 |
| ATOM | 774 | ND1 | HIS | 394 | 40.040 | -6.583 | 59.452 | 1.00 | 40.00 |
| ATOM | 776 | CE1 | HIS | 394 | 41.125 | -7.298 | 59.061 | 1.00 | 40.00 |
| ATOM | 777 | NE2 | HIS | 394 | 41.708 | -7.918 | 60.071 | 1.00 | 40.00 |
| ATOM | 779 | C | HIS | 394 | 40.542 | -4.479 | 62.140 | 1.00 | 40.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 780 | O | HIS | 394 | 41.183 | -4.881 | 63.110 | 1.00 | 40.00 |
| ATOM | 781 | N | ALA | 395 | 41.128 | -3.850 | 61.108 | 1.00 | 20.00 |
| ATOM | 783 | CA | ALA | 395 | 42.534 | -3.591 | 61.111 | 1.00 | 20.00 |
| ATOM | 784 | CB | ALA | 395 | 43.013 | -2.876 | 59.836 | 1.00 | 20.00 |
| ATOM | 785 | C | ALA | 395 | 42.905 | -2.722 | 62.278 | 1.00 | 20.00 |
| ATOM | 786 | O | ALA | 395 | 43.955 | -2.932 | 62.885 | 1.00 | 20.00 |
| ATOM | 787 | N | PHE | 396 | 42.069 | -1.717 | 62.626 | 1.00 | 20.00 |
| ATOM | 789 | CA | PHE | 396 | 42.434 | -0.830 | 63.705 | 1.00 | 20.00 |
| ATOM | 790 | CB | PHE | 396 | 41.987 | 0.623 | 63.471 | 1.00 | 20.00 |
| ATOM | 791 | CG | PHE | 396 | 42.601 | 1.137 | 62.215 | 1.00 | 20.00 |
| ATOM | 792 | CD1 | PHE | 396 | 41.970 | 0.936 | 61.010 | 1.00 | 20.00 |
| ATOM | 793 | CD2 | PHE | 396 | 43.750 | 1.892 | 62.249 | 1.00 | 20.00 |
| ATOM | 794 | CE1 | PHE | 396 | 42.471 | 1.484 | 59.854 | 1.00 | 20.00 |
| ATOM | 795 | CE2 | PHE | 396 | 44.253 | 2.448 | 61.097 | 1.00 | 20.00 |
| ATOM | 796 | CZ | PHE | 396 | 43.604 | 2.261 | 59.900 | 1.00 | 20.00 |
| ATOM | 797 | C | PHE | 396 | 41.763 | -1.229 | 64.987 | 1.00 | 20.00 |
| ATOM | 798 | O | PHE | 396 | 40.773 | -0.623 | 65.396 | 1.00 | 20.00 |
| ATOM | 799 | N | GLU | 397 | 42.341 | -2.208 | 65.703 | 1.00 | 20.00 |
| ATOM | 801 | CA | GLU | 397 | 41.757 | -2.723 | 66.905 | 1.00 | 20.00 |
| ATOM | 802 | CB | GLU | 397 | 42.569 | -3.905 | 67.471 | 1.00 | 20.00 |
| ATOM | 803 | CG | GLU | 397 | 41.904 | -4.650 | 68.632 | 1.00 | 20.00 |
| ATOM | 804 | CD | GLU | 397 | 42.496 | -4.154 | 69.944 | 1.00 | 20.00 |
| ATOM | 805 | OE1 | GLU | 397 | 42.958 | -2.984 | 69.989 | 1.00 | 20.00 |
| ATOM | 806 | OE2 | GLU | 397 | 42.499 | -4.948 | 70.923 | 1.00 | 20.00 |
| ATOM | 807 | C | GLU | 397 | 41.655 | -1.675 | 67.964 | 1.00 | 20.00 |
| ATOM | 808 | O | GLU | 397 | 40.644 | -1.605 | 68.659 | 1.00 | 20.00 |
| ATOM | 809 | N | ASN | 398 | 42.685 | -0.827 | 68.149 | 1.00 | 20.00 |
| ATOM | 811 | CA | ASN | 398 | 42.500 | 0.116 | 69.212 | 1.00 | 20.00 |
| ATOM | 812 | CB | ASN | 398 | 43.278 | -0.228 | 70.496 | 1.00 | 20.00 |
| ATOM | 813 | CG | ASN | 398 | 44.748 | -0.336 | 70.160 | 1.00 | 20.00 |
| ATOM | 814 | OD1 | ASN | 398 | 45.445 | 0.664 | 70.001 | 1.00 | 20.00 |
| ATOM | 815 | ND2 | ASN | 398 | 45.231 | -1.602 | 70.058 | 1.00 | 20.00 |
| ATOM | 818 | C | ASN | 398 | 42.762 | 1.538 | 68.839 | 1.00 | 20.00 |
| ATOM | 819 | O | ASN | 398 | 43.417 | 2.273 | 69.576 | 1.00 | 20.00 |
| ATOM | 820 | N | LEU | 399 | 42.217 | 1.979 | 67.692 | 1.00 | 20.00 |
| ATOM | 822 | CA | LEU | 399 | 42.347 | 3.356 | 67.321 | 1.00 | 20.00 |
| ATOM | 823 | CB | LEU | 399 | 41.827 | 3.606 | 65.897 | 1.00 | 20.00 |
| ATOM | 824 | CG | LEU | 399 | 41.928 | 5.058 | 65.406 | 1.00 | 20.00 |
| ATOM | 825 | CD1 | LEU | 399 | 43.391 | 5.505 | 65.279 | 1.00 | 20.00 |
| ATOM | 826 | CD2 | LEU | 399 | 41.127 | 5.245 | 64.106 | 1.00 | 20.00 |
| ATOM | 827 | C | LEU | 399 | 41.471 | 4.100 | 68.289 | 1.00 | 20.00 |
| ATOM | 828 | O | LEU | 399 | 40.256 | 3.918 | 68.277 | 1.00 | 20.00 |
| ATOM | 829 | N | GLU | 400 | 42.091 | 4.869 | 69.215 | 1.00 | 20.00 |
| ATOM | 831 | CA | GLU | 400 | 41.431 | 5.661 | 70.222 | 1.00 | 20.00 |
| ATOM | 832 | CB | GLU | 400 | 42.356 | 6.005 | 71.405 | 1.00 | 20.00 |
| ATOM | 833 | CG | GLU | 400 | 42.782 | 4.812 | 72.263 | 1.00 | 20.00 |
| ATOM | 834 | CD | GLU | 400 | 43.606 | 5.354 | 73.425 | 1.00 | 20.00 |
| ATOM | 835 | OE1 | GLU | 400 | 44.471 | 6.236 | 73.178 | 1.00 | 20.00 |
| ATOM | 836 | OE2 | GLU | 400 | 43.375 | 4.898 | 74.578 | 1.00 | 20.00 |
| ATOM | 837 | C | GLU | 400 | 40.825 | 6.981 | 69.817 | 1.00 | 20.00 |
| ATOM | 838 | O | GLU | 400 | 39.679 | 7.269 | 70.160 | 1.00 | 20.00 |
| ATOM | 839 | N | ILE | 401 | 41.572 | 7.832 | 69.077 | 1.00 | 20.00 |
| ATOM | 841 | CA | ILE | 401 | 41.078 | 9.168 | 68.850 | 1.00 | 20.00 |
| ATOM | 842 | CB | ILE | 401 | 41.695 | 10.146 | 69.819 | 1.00 | 20.00 |
| ATOM | 843 | CG2 | ILE | 401 | 43.157 | 10.343 | 69.395 | 1.00 | 20.00 |
| ATOM | 844 | CG1 | ILE | 401 | 40.914 | 11.465 | 69.932 | 1.00 | 20.00 |
| ATOM | 845 | CD1 | ILE | 401 | 39.739 | 11.393 | 70.906 | 1.00 | 20.00 |
| ATOM | 846 | C | ILE | 401 | 41.463 | 9.647 | 67.479 | 1.00 | 20.00 |
| ATOM | 847 | O | ILE | 401 | 42.510 | 9.275 | 66.952 | 1.00 | 20.00 |
| ATOM | 848 | N | ILE | 402 | 40.600 | 10.483 | 66.858 | 1.00 | 20.00 |
| ATOM | 850 | CA | ILE | 402 | 40.900 | 11.079 | 65.584 | 1.00 | 20.00 |
| ATOM | 851 | CB | ILE | 402 | 39.949 | 10.655 | 64.500 | 1.00 | 20.00 |
| ATOM | 852 | CG2 | ILE | 402 | 40.278 | 11.455 | 63.230 | 1.00 | 20.00 |
| ATOM | 853 | CG1 | ILE | 402 | 40.012 | 9.132 | 64.295 | 1.00 | 20.00 |

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|------|-----|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 854 | CD1 | ILE | 402 | 38.867 | 8.585 | 63.442 | 1.00 | 20.00 |
| ATOM | 855 | C | ILE | 402 | 40.704 | 12.546 | 65.815 | 1.00 | 20.00 |
| ATOM | 856 | O | ILE | 402 | 39.584 | 13.045 | 65.775 | 1.00 | 20.00 |
| ATOM | 857 | N | ARG | 403 | 41.806 | 13.295 | 65.984 | 1.00 | 20.00 |
| ATOM | 859 | CA | ARG | 403 | 41.738 | 14.672 | 66.393 | 1.00 | 20.00 |
| ATOM | 860 | CB | ARG | 403 | 43.121 | 15.317 | 66.557 | 1.00 | 20.00 |
| ATOM | 861 | CG | ARG | 403 | 43.868 | 14.804 | 67.785 | 1.00 | 20.00 |
| ATOM | 862 | CD | ARG | 403 | 45.126 | 15.607 | 68.111 | 1.00 | 20.00 |
| ATOM | 863 | NE | ARG | 403 | 45.666 | 15.072 | 69.390 | 1.00 | 20.00 |
| ATOM | 865 | CZ | ARG | 403 | 45.210 | 15.567 | 70.578 | 1.00 | 20.00 |
| ATOM | 866 | NH1 | ARG | 403 | 45.704 | 15.080 | 71.753 | 1.00 | 20.00 |
| ATOM | 869 | NH2 | ARG | 403 | 44.258 | 16.545 | 70.591 | 1.00 | 20.00 |
| ATOM | 872 | C | ARG | 403 | 40.944 | 15.560 | 65.491 | 1.00 | 20.00 |
| ATOM | 873 | O | ARG | 403 | 40.289 | 16.485 | 65.964 | 1.00 | 20.00 |
| ATOM | 874 | N | GLY | 404 | 40.997 | 15.347 | 64.168 | 1.00 | 20.00 |
| ATOM | 876 | CA | GLY | 404 | 40.235 | 16.191 | 63.295 | 1.00 | 20.00 |
| ATOM | 877 | C | GLY | 404 | 40.869 | 17.541 | 63.176 | 1.00 | 20.00 |
| ATOM | 878 | O | GLY | 404 | 40.188 | 18.528 | 62.898 | 1.00 | 20.00 |
| ATOM | 879 | N | ARG | 405 | 42.199 | 17.625 | 63.364 | 1.00 | 20.00 |
| ATOM | 881 | CA | ARG | 405 | 42.834 | 18.908 | 63.279 | 1.00 | 20.00 |
| ATOM | 882 | CB | ARG | 405 | 44.355 | 18.861 | 63.503 | 1.00 | 20.00 |
| ATOM | 883 | CG | ARG | 405 | 44.950 | 20.250 | 63.742 | 1.00 | 20.00 |
| ATOM | 884 | CD | ARG | 405 | 46.470 | 20.259 | 63.903 | 1.00 | 20.00 |
| ATOM | 885 | NE | ARG | 405 | 47.048 | 20.241 | 62.532 | 1.00 | 20.00 |
| ATOM | 887 | CZ | ARG | 405 | 47.194 | 21.412 | 61.846 | 1.00 | 20.00 |
| ATOM | 888 | NH1 | ARG | 405 | 46.838 | 22.594 | 62.429 | 1.00 | 20.00 |
| ATOM | 891 | NH2 | ARG | 405 | 47.689 | 21.400 | 60.574 | 1.00 | 20.00 |
| ATOM | 894 | C | ARG | 405 | 42.576 | 19.416 | 61.898 | 1.00 | 20.00 |
| ATOM | 895 | O | ARG | 405 | 42.315 | 20.602 | 61.697 | 1.00 | 20.00 |
| ATOM | 896 | N | THR | 406 | 42.645 | 18.516 | 60.902 | 1.00 | 20.00 |
| ATOM | 898 | CA | THR | 406 | 42.323 | 18.902 | 59.561 | 1.00 | 20.00 |
| ATOM | 899 | CB | THR | 406 | 43.479 | 18.799 | 58.610 | 1.00 | 20.00 |
| ATOM | 900 | CG1 | THR | 406 | 43.939 | 17.459 | 58.535 | 1.00 | 20.00 |
| ATOM | 902 | CG2 | THR | 406 | 44.604 | 19.723 | 59.109 | 1.00 | 20.00 |
| ATOM | 903 | C | THR | 406 | 41.261 | 17.949 | 59.121 | 1.00 | 20.00 |
| ATOM | 904 | O | THR | 406 | 41.354 | 16.748 | 59.368 | 1.00 | 20.00 |
| ATOM | 905 | N | LYS | 407 | 40.218 | 18.467 | 58.449 | 1.00 | 20.00 |
| ATOM | 907 | CA | LYS | 407 | 39.097 | 17.653 | 58.078 | 1.00 | 20.00 |
| ATOM | 908 | CB | LYS | 407 | 37.788 | 18.227 | 58.638 | 1.00 | 20.00 |
| ATOM | 909 | CG | LYS | 407 | 37.577 | 19.672 | 58.180 | 1.00 | 20.00 |
| ATOM | 910 | CD | LYS | 407 | 36.235 | 20.287 | 58.571 | 1.00 | 20.00 |
| ATOM | 911 | CE | LYS | 407 | 36.072 | 21.725 | 58.076 | 1.00 | 20.00 |
| ATOM | 912 | NZ | LYS | 407 | 37.081 | 22.597 | 58.716 | 1.00 | 20.00 |
| ATOM | 916 | C | LYS | 407 | 38.962 | 17.595 | 56.591 | 1.00 | 20.00 |
| ATOM | 917 | O | LYS | 407 | 39.427 | 18.483 | 55.878 | 1.00 | 20.00 |
| ATOM | 918 | N | GLN | 408 | 38.330 | 16.518 | 56.080 | 1.00 | 20.00 |
| ATOM | 920 | CA | GLN | 408 | 38.139 | 16.441 | 54.663 | 1.00 | 20.00 |
| ATOM | 921 | CB | GLN | 408 | 38.080 | 15.016 | 54.076 | 1.00 | 20.00 |
| ATOM | 922 | CG | GLN | 408 | 36.898 | 14.167 | 54.539 | 1.00 | 20.00 |
| ATOM | 923 | CD | GLN | 408 | 36.969 | 12.853 | 53.772 | 1.00 | 20.00 |
| ATOM | 924 | OE1 | GLN | 408 | 36.014 | 12.455 | 53.107 | 1.00 | 20.00 |
| ATOM | 925 | NE2 | GLN | 408 | 38.139 | 12.164 | 53.857 | 1.00 | 20.00 |
| ATOM | 928 | C | GLN | 408 | 36.847 | 17.130 | 54.381 | 1.00 | 20.00 |
| ATOM | 929 | O | GLN | 408 | 36.081 | 17.408 | 55.301 | 1.00 | 20.00 |
| ATOM | 930 | N | HIS | 409 | 36.585 | 17.409 | 53.086 | 1.00 | 20.00 |
| ATOM | 932 | CA | HIS | 409 | 35.431 | 18.151 | 52.662 | 1.00 | 20.00 |
| ATOM | 933 | CB | HIS | 409 | 35.166 | 18.082 | 51.145 | 1.00 | 20.00 |
| ATOM | 934 | CG | HIS | 409 | 36.230 | 18.712 | 50.294 | 1.00 | 20.00 |
| ATOM | 935 | CD2 | HIS | 409 | 37.316 | 18.149 | 49.695 | 1.00 | 20.00 |
| ATOM | 936 | ND1 | HIS | 409 | 36.251 | 20.042 | 49.936 | 1.00 | 20.00 |
| ATOM | 938 | CE1 | HIS | 409 | 37.341 | 20.217 | 49.146 | 1.00 | 20.00 |
| ATOM | 939 | NE2 | HIS | 409 | 38.018 | 19.097 | 48.972 | 1.00 | 20.00 |
| ATOM | 941 | C | HIS | 409 | 34.216 | 17.607 | 53.323 | 1.00 | 20.00 |
| ATOM | 942 | O | HIS | 409 | 34.102 | 16.405 | 53.551 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 943 | N | GLY | 410 | 33.280 | 18.503 | 53.673 | 1.00 | 20.00 |
| ATOM | 945 | CA | GLY | 410 | 32.100 | 18.067 | 54.349 | 1.00 | 20.00 |
| ATOM | 946 | C | GLY | 410 | 32.429 | 18.116 | 55.801 | 1.00 | 20.00 |
| ATOM | 947 | O | GLY | 410 | 31.585 | 17.843 | 56.654 | 1.00 | 20.00 |
| ATOM | 948 | N | GLN | 411 | 33.681 | 18.501 | 56.113 | 1.00 | 20.00 |
| ATOM | 950 | CA | GLN | 411 | 34.103 | 18.580 | 57.477 | 1.00 | 20.00 |
| ATOM | 951 | CB | GLN | 411 | 33.207 | 19.505 | 58.319 | 1.00 | 20.00 |
| ATOM | 952 | CG | GLN | 411 | 33.226 | 20.973 | 57.890 | 1.00 | 20.00 |
| ATOM | 953 | CD | GLN | 411 | 32.231 | 21.722 | 58.767 | 1.00 | 20.00 |
| ATOM | 954 | OE1 | GLN | 411 | 31.032 | 21.444 | 58.750 | 1.00 | 20.00 |
| ATOM | 955 | NE2 | GLN | 411 | 32.742 | 22.699 | 59.562 | 1.00 | 20.00 |
| ATOM | 958 | C | GLN | 411 | 34.038 | 17.226 | 58.105 | 1.00 | 20.00 |
| ATOM | 959 | O | GLN | 411 | 33.609 | 17.101 | 59.250 | 1.00 | 20.00 |
| ATOM | 960 | N | PHE | 412 | 34.488 | 16.174 | 57.393 | 1.00 | 20.00 |
| ATOM | 962 | CA | PHE | 412 | 34.372 | 14.865 | 57.966 | 1.00 | 20.00 |
| ATOM | 963 | CB | PHE | 412 | 33.979 | 13.774 | 56.952 | 1.00 | 20.00 |
| ATOM | 964 | CG | PHE | 412 | 32.657 | 14.127 | 56.359 | 1.00 | 20.00 |
| ATOM | 965 | CD1 | PHE | 412 | 32.590 | 14.732 | 55.125 | 1.00 | 20.00 |
| ATOM | 966 | CD2 | PHE | 412 | 31.494 | 13.933 | 57.068 | 1.00 | 20.00 |
| ATOM | 967 | CE1 | PHE | 412 | 31.377 | 15.086 | 54.582 | 1.00 | 20.00 |
| ATOM | 968 | CE2 | PHE | 412 | 30.279 | 14.300 | 56.538 | 1.00 | 20.00 |
| ATOM | 969 | CZ | PHE | 412 | 30.217 | 14.866 | 55.287 | 1.00 | 20.00 |
| ATOM | 970 | C | PHE | 412 | 35.665 | 14.421 | 58.576 | 1.00 | 20.00 |
| ATOM | 971 | O | PHE | 412 | 36.735 | 14.549 | 57.986 | 1.00 | 20.00 |
| ATOM | 972 | N | SER | 413 | 35.579 | 13.964 | 59.837 | 1.00 | 20.00 |
| ATOM | 974 | CA | SER | 413 | 36.652 | 13.395 | 60.599 | 1.00 | 20.00 |
| ATOM | 975 | CB | SER | 413 | 36.267 | 13.239 | 62.073 | 1.00 | 20.00 |
| ATOM | 976 | OG | SER | 413 | 35.611 | 14.412 | 62.523 | 1.00 | 20.00 |
| ATOM | 978 | C | SER | 413 | 36.871 | 12.000 | 60.127 | 1.00 | 20.00 |
| ATOM | 979 | O | SER | 413 | 38.002 | 11.534 | 60.023 | 1.00 | 20.00 |
| ATOM | 980 | N | LEU | 414 | 35.754 | 11.288 | 59.881 | 1.00 | 20.00 |
| ATOM | 982 | CA | LEU | 414 | 35.805 | 9.915 | 59.483 | 1.00 | 20.00 |
| ATOM | 983 | CB | LEU | 414 | 35.290 | 8.979 | 60.592 | 1.00 | 20.00 |
| ATOM | 984 | CG | LEU | 414 | 35.304 | 7.480 | 60.252 | 1.00 | 20.00 |
| ATOM | 985 | CD1 | LEU | 414 | 36.732 | 6.966 | 60.018 | 1.00 | 20.00 |
| ATOM | 986 | CD2 | LEU | 414 | 34.543 | 6.670 | 61.315 | 1.00 | 20.00 |
| ATOM | 987 | C | LEU | 414 | 34.909 | 9.756 | 58.304 | 1.00 | 20.00 |
| ATOM | 988 | O | LEU | 414 | 33.688 | 9.855 | 58.414 | 1.00 | 20.00 |
| ATOM | 989 | N | ALA | 415 | 35.501 | 9.503 | 57.126 | 1.00 | 20.00 |
| ATOM | 991 | CA | ALA | 415 | 34.678 | 9.310 | 55.973 | 1.00 | 20.00 |
| ATOM | 992 | CB | ALA | 415 | 35.070 | 10.198 | 54.779 | 1.00 | 20.00 |
| ATOM | 993 | C | ALA | 415 | 34.858 | 7.893 | 55.551 | 1.00 | 20.00 |
| ATOM | 994 | O | ALA | 415 | 35.981 | 7.453 | 55.314 | 1.00 | 20.00 |
| ATOM | 995 | N | VAL | 416 | 33.750 | 7.129 | 55.490 | 1.00 | 20.00 |
| ATOM | 997 | CA | VAL | 416 | 33.822 | 5.776 | 55.025 | 1.00 | 20.00 |
| ATOM | 998 | CB | VAL | 416 | 33.376 | 4.767 | 56.042 | 1.00 | 20.00 |
| ATOM | 999 | CG1 | VAL | 416 | 33.451 | 3.368 | 55.405 | 1.00 | 20.00 |
| ATOM | 1000 | CG2 | VAL | 416 | 34.245 | 4.921 | 57.301 | 1.00 | 20.00 |
| ATOM | 1001 | C | VAL | 416 | 32.869 | 5.702 | 53.878 | 1.00 | 20.00 |
| ATOM | 1002 | O | VAL | 416 | 31.655 | 5.739 | 54.068 | 1.00 | 20.00 |
| ATOM | 1003 | N | VAL | 417 | 33.392 | 5.581 | 52.645 | 1.00 | 20.00 |
| ATOM | 1005 | CA | VAL | 417 | 32.503 | 5.564 | 51.522 | 1.00 | 20.00 |
| ATOM | 1006 | CB | VAL | 417 | 32.770 | 6.667 | 50.541 | 1.00 | 20.00 |
| ATOM | 1007 | CG1 | VAL | 417 | 31.784 | 6.531 | 49.369 | 1.00 | 20.00 |
| ATOM | 1008 | CG2 | VAL | 417 | 32.682 | 8.013 | 51.277 | 1.00 | 20.00 |
| ATOM | 1009 | C | VAL | 417 | 32.669 | 4.279 | 50.779 | 1.00 | 20.00 |
| ATOM | 1010 | O | VAL | 417 | 33.789 | 3.805 | 50.597 | 1.00 | 20.00 |
| ATOM | 1011 | N | SER | 418 | 31.533 | 3.706 | 50.321 | 1.00 | 40.00 |
| ATOM | 1013 | CA | SER | 418 | 31.494 | 2.482 | 49.564 | 1.00 | 40.00 |
| ATOM | 1014 | CB | SER | 418 | 31.778 | 2.690 | 48.065 | 1.00 | 40.00 |
| ATOM | 1015 | OG | SER | 418 | 33.087 | 3.207 | 47.882 | 1.00 | 40.00 |
| ATOM | 1017 | C | SER | 418 | 32.463 | 1.474 | 50.101 | 1.00 | 40.00 |
| ATOM | 1018 | O | SER | 418 | 33.596 | 1.381 | 49.632 | 1.00 | 40.00 |
| ATOM | 1019 | N | LEU | 419 | 32.040 | 0.703 | 51.124 | 1.00 | 40.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| A | 1021 | CA | LEU | 419 | 32.930 | -0.252 | 51.727 | 1.00 | 40.00 |
| ATOM | 1022 | CB | LEU | 419 | 33.355 | 0.212 | 53.133 | 1.00 | 40.00 |
| ATOM | 1023 | CG | LEU | 419 | 34.471 | -0.608 | 53.800 | 1.00 | 40.00 |
| 1 4 | 1024 | CD1 | LEU | 419 | 35.781 | -0.502 | 53.005 | 1.00 | 40.00 |
| ATOM | 1025 | CD2 | LEU | 419 | 34.654 | -0.187 | 55.267 | 1.00 | 40.00 |
| ATOM | 1026 | C | LEU | 419 | 32.191 | -1.562 | 51.860 | 1.00 | 40.00 |
| ATOM | 1027 | O | LEU | 419 | 30.971 | -1.567 | 51.980 | 1.00 | 40.00 |
| ATOM | 1028 | N | ASN | 420 | 32.888 | -2.724 | 51.824 | 1.00 | 40.00 |
| ATOM | 1030 | CA | ASN | 420 | 32.176 | -3.970 | 51.957 | 1.00 | 40.00 |
| ATOM | 1031 | CB | ASN | 420 | 32.676 | -5.083 | 51.022 | 1.00 | 40.00 |
| ATOM | 1032 | CG | ASN | 420 | 32.133 | -4.765 | 49.636 | 1.00 | 40.00 |
| ATOM | 1033 | OD1 | ASN | 420 | 32.655 | -5.225 | 48.622 | 1.00 | 40.00 |
| ATOM | 1034 | ND2 | ASN | 420 | 31.047 | -3.946 | 49.591 | 1.00 | 40.00 |
| ATOM | 1037 | C | ASN | 420 | 32.296 | -4.436 | 53.366 | 1.00 | 40.00 |
| ATOM | 1038 | O | ASN | 420 | 32.839 | -5.503 | 53.642 | 1.00 | 40.00 |
| ATOM | 1039 | N | ILE | 421 | 31.756 | -3.654 | 54.316 | 1.00 | 40.00 |
| ATOM | 1041 | CA | ILE | 421 | 31.927 | -4.069 | 55.669 | 1.00 | 40.00 |
| ATOM | 1042 | CB | ILE | 421 | 32.813 | -3.154 | 56.450 | 1.00 | 40.00 |
| ATOM | 1043 | CG2 | ILE | 421 | 32.914 | -3.688 | 57.888 | 1.00 | 40.00 |
| ATOM | 1044 | CG1 | ILE | 421 | 34.165 | -3.055 | 55.728 | 1.00 | 40.00 |
| ATOM | 1045 | CD1 | ILE | 421 | 34.783 | -4.417 | 55.417 | 1.00 | 40.00 |
| ATOM | 1046 | C | ILE | 421 | 30.629 | -4.187 | 56.387 | 1.00 | 40.00 |
| ATOM | 1047 | O | ILE | 421 | 29.675 | -3.461 | 56.115 | 1.00 | 40.00 |
| ATOM | 1048 | N | THR | 422 | 30.572 | -5.185 | 57.289 | 1.00 | 40.00 |
| ATOM | 1050 | CA | THR | 422 | 29.453 | -5.479 | 58.131 | 1.00 | 40.00 |
| ATOM | 1051 | CB | THR | 422 | 29.559 | -6.840 | 58.751 | 1.00 | 40.00 |
| ATOM | 1052 | OG1 | THR | 422 | 30.720 | -6.920 | 59.564 | 1.00 | 40.00 |
| ATOM | 1054 | CG2 | THR | 422 | 29.628 | -7.884 | 57.622 | 1.00 | 40.00 |
| ATOM | 1055 | C | THR | 422 | 29.301 | -4.487 | 59.241 | 1.00 | 40.00 |
| ATOM | 1056 | O | THR | 422 | 28.183 | -4.130 | 59.601 | 1.00 | 40.00 |
| ATOM | 1057 | N | SER | 423 | 30.416 | -4.022 | 59.842 | 1.00 | 20.00 |
| ATOM | 1059 | CA | SER | 423 | 30.266 | -3.123 | 60.951 | 1.00 | 20.00 |
| ATOM | 1060 | CB | SER | 423 | 30.124 | -3.861 | 62.296 | 1.00 | 20.00 |
| ATOM | 1061 | OG | SER | 423 | 29.972 | -2.937 | 63.364 | 1.00 | 20.00 |
| ATOM | 1063 | C | SER | 423 | 31.482 | -2.254 | 61.046 | 1.00 | 20.00 |
| ATOM | 1064 | O | SER | 423 | 32.423 | -2.422 | 60.273 | 1.00 | 20.00 |
| ATOM | 1065 | N | LEU | 424 | 31.436 | -1.238 | 61.938 | 1.00 | 20.00 |
| ATOM | 1067 | CA | LEU | 424 | 32.556 | -0.374 | 62.194 | 1.00 | 20.00 |
| ATOM | 1068 | CB | LEU | 424 | 32.159 | 0.841 | 63.054 | 1.00 | 20.00 |
| ATOM | 1069 | CG | LEU | 424 | 31.078 | 1.743 | 62.419 | 1.00 | 20.00 |
| ATOM | 1070 | CD1 | LEU | 424 | 31.575 | 2.391 | 61.116 | 1.00 | 20.00 |
| ATOM | 1071 | CD2 | LEU | 424 | 29.741 | 1.001 | 62.254 | 1.00 | 20.00 |
| ATOM | 1072 | C | LEU | 424 | 33.616 | -1.131 | 62.947 | 1.00 | 20.00 |
| ATOM | 1073 | O | LEU | 424 | 34.764 | -1.191 | 62.523 | 1.00 | 20.00 |
| ATOM | 1074 | N | GLY | 425 | 33.269 | -1.752 | 64.093 | 1.00 | 20.00 |
| ATOM | 1076 | CA | GLY | 425 | 34.242 | -2.537 | 64.818 | 1.00 | 20.00 |
| ATOM | 1077 | C | GLY | 425 | 35.328 | -1.708 | 65.458 | 1.00 | 20.00 |
| ATOM | 1078 | O | GLY | 425 | 36.307 | -2.237 | 65.980 | 1.00 | 20.00 |
| ATOM | 1079 | N | LEU | 426 | 35.143 | -0.381 | 65.462 | 1.00 | 20.00 |
| ATOM | 1081 | CA | LEU | 426 | 36.012 | 0.656 | 65.963 | 1.00 | 20.00 |
| ATOM | 1082 | CB | LEU | 426 | 35.706 | 2.062 | 65.412 | 1.00 | 20.00 |
| ATOM | 1083 | CG | LEU | 426 | 36.084 | 2.249 | 63.931 | 1.00 | 20.00 |
| ATOM | 1084 | CD1 | LEU | 426 | 35.790 | 3.681 | 63.458 | 1.00 | 20.00 |
| ATOM | 1085 | CD2 | LEU | 426 | 37.542 | 1.836 | 63.676 | 1.00 | 20.00 |
| ATOM | 1086 | C | LEU | 426 | 35.965 | 0.746 | 67.452 | 1.00 | 20.00 |
| ATOM | 1087 | O | LEU | 426 | 36.277 | 1.801 | 67.987 | 1.00 | 20.00 |
| ATOM | 1088 | N | ARG | 427 | 35.524 | -0.305 | 68.168 | 1.00 | 20.00 |
| ATOM | 1090 | CA | ARG | 427 | 35.179 | -0.216 | 69.568 | 1.00 | 20.00 |
| ATOM | 1091 | CB | ARG | 427 | 35.061 | -1.583 | 70.265 | 1.00 | 20.00 |
| ATOM | 1092 | CG | ARG | 427 | 36.373 | -2.362 | 70.329 | 1.00 | 20.00 |
| ATOM | 1093 | CD | ARG | 427 | 36.329 | -3.537 | 71.307 | 1.00 | 20.00 |
| ATOM | 1094 | NE | ARG | 427 | 37.689 | -4.143 | 71.322 | 1.00 | 20.00 |
| ATOM | 1096 | CZ | ARG | 427 | 38.665 | -3.598 | 72.105 | 1.00 | 20.00 |
| ATOM | 1097 | NH1 | ARG | 427 | 38.390 | -2.515 | 72.890 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1100 | NH2 | ARG | 427 | 39.924 | -4.125 | 72.091 | 1.00 | 20.00 |
| ATOM | 1103 | C | ARG | 427 | 36.081 | 0.609 | 70.444 | 1.00 | 20.00 |
| ATOM | 1104 | O | ARG | 427 | 35.606 | 1.179 | 71.423 | 1.00 | 20.00 |
| M | 1105 | N | SER | 428 | 37.393 | 0.670 | 70.174 | 1.00 | 20.00 |
| ATOM | 1107 | CA | SER | 428 | 38.285 | 1.469 | 70.974 | 1.00 | 20.00 |
| ATOM | 1108 | CB | SER | 428 | 39.760 | 1.196 | 70.643 | 1.00 | 20.00 |
| ATOM | 1109 | OG | SER | 428 | 40.020 | 1.553 | 69.294 | 1.00 | 20.00 |
| ATOM | 1111 | C | SER | 428 | 38.056 | 2.952 | 70.818 | 1.00 | 20.00 |
| ATOM | 1112 | O | SER | 428 | 38.444 | 3.741 | 71.677 | 1.00 | 20.00 |
| ATOM | 1113 | N | LEU | 429 | 37.456 | 3.375 | 69.690 | 1.00 | 20.00 |
| ATOM | 1115 | CA | LEU | 429 | 37.291 | 4.759 | 69.331 | 1.00 | 20.00 |
| ATOM | 1116 | CB | LEU | 429 | 36.679 | 4.907 | 67.924 | 1.00 | 20.00 |
| ATOM | 1117 | CG | LEU | 429 | 36.534 | 6.355 | 67.423 | 1.00 | 20.00 |
| ATOM | 1118 | CD1 | LEU | 429 | 37.911 | 7.015 | 67.237 | 1.00 | 20.00 |
| ATOM | 1119 | CD2 | LEU | 429 | 35.668 | 6.419 | 66.152 | 1.00 | 20.00 |
| ATOM | 1120 | C | LEU | 429 | 36.441 | 5.523 | 70.302 | 1.00 | 20.00 |
| ATOM | 1121 | O | LEU | 429 | 35.213 | 5.440 | 70.285 | 1.00 | 20.00 |
| ATOM | 1122 | N | LYS | 430 | 37.105 | 6.242 | 71.230 | 1.00 | 20.00 |
| ATOM | 1124 | CA | LYS | 430 | 36.429 | 7.073 | 72.178 | 1.00 | 20.00 |
| ATOM | 1125 | CB | LYS | 430 | 37.263 | 7.316 | 73.436 | 1.00 | 20.00 |
| ATOM | 1126 | CG | LYS | 430 | 37.388 | 6.040 | 74.265 | 1.00 | 20.00 |
| ATOM | 1127 | CD | LYS | 430 | 38.410 | 6.146 | 75.388 | 1.00 | 20.00 |
| ATOM | 1128 | CE | LYS | 430 | 38.325 | 4.996 | 76.391 | 1.00 | 20.00 |
| ATOM | 1129 | NZ | LYS | 430 | 39.167 | 5.291 | 77.572 | 1.00 | 20.00 |
| ATOM | 1133 | C | LYS | 430 | 35.960 | 8.392 | 71.653 | 1.00 | 20.00 |
| ATOM | 1134 | O | LYS | 430 | 34.829 | 8.788 | 71.920 | 1.00 | 20.00 |
| ATOM | 1135 | N | GLU | 431 | 36.797 | 9.134 | 70.896 | 1.00 | 20.00 |
| ATOM | 1137 | CA | GLU | 431 | 36.277 | 10.402 | 70.477 | 1.00 | 20.00 |
| ATOM | 1138 | CB | GLU | 431 | 36.374 | 11.497 | 71.552 | 1.00 | 20.00 |
| ATOM | 1139 | CG | GLU | 431 | 35.636 | 12.776 | 71.151 | 1.00 | 20.00 |
| ATOM | 1140 | CD | GLU | 431 | 35.614 | 13.725 | 72.339 | 1.00 | 20.00 |
| ATOM | 1141 | OE1 | GLU | 431 | 36.713 | 14.064 | 72.853 | 1.00 | 20.00 |
| ATOM | 1142 | OE2 | GLU | 431 | 34.491 | 14.125 | 72.749 | 1.00 | 20.00 |
| ATOM | 1143 | C | GLU | 431 | 36.920 | 10.936 | 69.242 | 1.00 | 20.00 |
| ATOM | 1144 | O | GLU | 431 | 38.056 | 10.606 | 68.902 | 1.00 | 20.00 |
| ATOM | 1145 | N | ILE | 432 | 36.155 | 11.771 | 68.512 | 1.00 | 20.00 |
| ATOM | 1147 | CA | ILE | 432 | 36.674 | 12.438 | 67.363 | 1.00 | 20.00 |
| ATOM | 1148 | CB | ILE | 432 | 35.882 | 12.180 | 66.111 | 1.00 | 20.00 |
| ATOM | 1149 | CG2 | ILE | 432 | 36.343 | 13.160 | 65.021 | 1.00 | 20.00 |
| ATOM | 1150 | CG1 | ILE | 432 | 36.042 | 10.697 | 65.719 | 1.00 | 20.00 |
| ATOM | 1151 | CD1 | ILE | 432 | 35.157 | 10.240 | 64.561 | 1.00 | 20.00 |
| ATOM | 1152 | C | ILE | 432 | 36.637 | 13.880 | 67.732 | 1.00 | 20.00 |
| ATOM | 1153 | O | ILE | 432 | 35.638 | 14.574 | 67.562 | 1.00 | 20.00 |
| ATOM | 1154 | N | SER | 433 | 37.801 | 14.387 | 68.155 | 1.00 | 20.00 |
| ATOM | 1156 | CA | SER | 433 | 37.934 | 15.679 | 68.751 | 1.00 | 20.00 |
| ATOM | 1157 | CB | SER | 433 | 39.413 | 16.039 | 68.966 | 1.00 | 20.00 |
| ATOM | 1158 | OG | SER | 433 | 39.525 | 17.269 | 69.660 | 1.00 | 20.00 |
| ATOM | 1160 | C | SER | 433 | 37.297 | 16.746 | 67.915 | 1.00 | 20.00 |
| ATOM | 1161 | O | SER | 433 | 36.732 | 17.688 | 68.465 | 1.00 | 20.00 |
| ATOM | 1162 | N | ASP | 434 | 37.373 | 16.661 | 66.574 | 1.00 | 20.00 |
| ATOM | 1164 | CA | ASP | 434 | 36.769 | 17.708 | 65.793 | 1.00 | 20.00 |
| ATOM | 1165 | CB | ASP | 434 | 37.778 | 18.757 | 65.285 | 1.00 | 20.00 |
| ATOM | 1166 | CG | ASP | 434 | 38.367 | 19.559 | 66.437 | 1.00 | 20.00 |
| ATOM | 1167 | OD1 | ASP | 434 | 39.564 | 19.935 | 66.325 | 1.00 | 20.00 |
| ATOM | 1168 | OD2 | ASP | 434 | 37.636 | 19.820 | 67.428 | 1.00 | 20.00 |
| ATOM | 1169 | C | ASP | 434 | 36.205 | 17.125 | 64.536 | 1.00 | 20.00 |
| ATOM | 1170 | O | ASP | 434 | 36.755 | 16.164 | 64.006 | 1.00 | 20.00 |
| ATOM | 1171 | N | GLY | 435 | 35.099 | 17.712 | 64.023 | 1.00 | 20.00 |
| ATOM | 1173 | CA | GLY | 435 | 34.518 | 17.298 | 62.776 | 1.00 | 20.00 |
| ATOM | 1174 | C | GLY | 435 | 33.489 | 16.239 | 63.009 | 1.00 | 20.00 |
| ATOM | 1175 | O | GLY | 435 | 33.406 | 15.670 | 64.096 | 1.00 | 20.00 |
| ATOM | 1176 | N | ASP | 436 | 32.666 | 15.958 | 61.972 | 1.00 | 20.00 |
| ATOM | 1178 | CA | ASP | 436 | 31.658 | 14.941 | 62.091 | 1.00 | 20.00 |
| ATOM | 1179 | CB | ASP | 436 | 30.248 | 15.361 | 61.626 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1180 | CG | ASP | 436 | 30.254 | 15.669 | 60.138 | 1.00 | 20.00 |
| ATOM | 1181 | OD1 | ASP | 436 | 31.256 | 16.260 | 59.658 | 1.00 | 20.00 |
| ATOM | 1182 | OD2 | ASP | 436 | 29.252 | 15.318 | 59.459 | 1.00 | 20.00 |
| ATOM | 1183 | C | ASP | 436 | 32.073 | 13.745 | 61.293 | 1.00 | 20.00 |
| ATOM | 1184 | O | ASP | 436 | 33.236 | 13.617 | 60.924 | 1.00 | 20.00 |
| ATOM | 1185 | N | VAL | 437 | 31.138 | 12.805 | 61.036 | 1.00 | 20.00 |
| ATOM | 1187 | CA | VAL | 437 | 31.480 | 11.636 | 60.270 | 1.00 | 20.00 |
| ATOM | 1188 | CB | VAL | 437 | 31.538 | 10.383 | 61.101 | 1.00 | 20.00 |
| ATOM | 1189 | CG1 | VAL | 437 | 31.609 | 9.134 | 60.207 | 1.00 | 20.00 |
| ATOM | 1190 | CG2 | VAL | 437 | 32.787 | 10.510 | 61.984 | 1.00 | 20.00 |
| ATOM | 1191 | C | VAL | 437 | 30.518 | 11.447 | 59.139 | 1.00 | 20.00 |
| ATOM | 1192 | O | VAL | 437 | 29.386 | 11.919 | 59.199 | 1.00 | 20.00 |
| ATOM | 1193 | N | ILE | 438 | 30.965 | 10.802 | 58.037 | 1.00 | 20.00 |
| ATOM | 1195 | CA | ILE | 438 | 30.073 | 10.553 | 56.944 | 1.00 | 20.00 |
| ATOM | 1196 | CB | ILE | 438 | 30.382 | 11.398 | 55.726 | 1.00 | 20.00 |
| ATOM | 1197 | CG2 | ILE | 438 | 31.787 | 11.046 | 55.207 | 1.00 | 20.00 |
| ATOM | 1198 | CG1 | ILE | 438 | 29.259 | 11.328 | 54.670 | 1.00 | 20.00 |
| ATOM | 1199 | CD1 | ILE | 438 | 29.073 | 9.964 | 54.005 | 1.00 | 20.00 |
| ATOM | 1200 | C | ILE | 438 | 30.118 | 9.092 | 56.609 | 1.00 | 20.00 |
| ATOM | 1201 | O | ILE | 438 | 31.115 | 8.561 | 56.122 | 1.00 | 20.00 |
| ATOM | 1202 | N | ILE | 439 | 29.012 | 8.381 | 56.877 | 1.00 | 20.00 |
| ATOM | 1204 | CA | ILE | 439 | 29.001 | 6.988 | 56.549 | 1.00 | 20.00 |
| ATOM | 1205 | CB | ILE | 439 | 28.507 | 6.134 | 57.681 | 1.00 | 20.00 |
| ATOM | 1206 | CG2 | ILE | 439 | 28.420 | 4.677 | 57.195 | 1.00 | 20.00 |
| ATOM | 1207 | CG1 | ILE | 439 | 29.412 | 6.316 | 58.910 | 1.00 | 20.00 |
| ATOM | 1208 | CD1 | ILE | 439 | 28.821 | 5.723 | 60.188 | 1.00 | 20.00 |
| ATOM | 1209 | C | ILE | 439 | 28.042 | 6.847 | 55.410 | 1.00 | 20.00 |
| ATOM | 1210 | O | ILE | 439 | 26.831 | 6.784 | 55.614 | 1.00 | 20.00 |
| ATOM | 1211 | N | SER | 440 | 28.563 | 6.770 | 54.167 | 1.00 | 20.00 |
| ATOM | 1213 | CA | SER | 440 | 27.669 | 6.726 | 53.047 | 1.00 | 20.00 |
| ATOM | 1214 | CB | SER | 440 | 27.725 | 8.001 | 52.186 | 1.00 | 20.00 |
| ATOM | 1215 | OG | SER | 440 | 26.819 | 7.899 | 51.097 | 1.00 | 20.00 |
| ATOM | 1217 | C | SER | 440 | 27.936 | 5.571 | 52.133 | 1.00 | 20.00 |
| ATOM | 1218 | O | SER | 440 | 29.056 | 5.070 | 52.032 | 1.00 | 20.00 |
| ATOM | 1219 | N | GLY | 441 | 26.867 | 5.109 | 51.455 | 1.00 | 20.00 |
| ATOM | 1221 | CA | GLY | 441 | 26.962 | 4.082 | 50.458 | 1.00 | 20.00 |
| ATOM | 1222 | C | GLY | 441 | 27.610 | 2.838 | 50.970 | 1.00 | 20.00 |
| ATOM | 1223 | O | GLY | 441 | 28.639 | 2.420 | 50.440 | 1.00 | 20.00 |
| ATOM | 1224 | N | ASN | 442 | 27.056 | 2.230 | 52.037 | 1.00 | 20.00 |
| ATOM | 1226 | CA | ASN | 442 | 27.610 | 0.991 | 52.508 | 1.00 | 20.00 |
| ATOM | 1227 | CB | ASN | 442 | 28.298 | 1.143 | 53.873 | 1.00 | 20.00 |
| ATOM | 1228 | CG | ASN | 442 | 29.495 | 2.061 | 53.665 | 1.00 | 20.00 |
| ATOM | 1229 | OD1 | ASN | 442 | 30.454 | 1.711 | 52.979 | 1.00 | 20.00 |
| ATOM | 1230 | ND2 | ASN | 442 | 29.430 | 3.282 | 54.259 | 1.00 | 20.00 |
| ATOM | 1233 | C | ASN | 442 | 26.463 | 0.049 | 52.672 | 1.00 | 20.00 |
| ATOM | 1234 | O | ASN | 442 | 25.955 | -0.145 | 53.775 | 1.00 | 20.00 |
| ATOM | 1235 | N | LYS | 443 | 26.091 | -0.654 | 51.589 | 1.00 | 20.00 |
| ATOM | 1237 | CA | LYS | 443 | 24.876 | -1.410 | 51.620 | 1.00 | 20.00 |
| ATOM | 1238 | CB | LYS | 443 | 24.582 | -2.098 | 50.279 | 1.00 | 20.00 |
| ATOM | 1239 | CG | LYS | 443 | 24.381 | -1.055 | 49.178 | 1.00 | 20.00 |
| ATOM | 1240 | CD | LYS | 443 | 23.303 | -0.027 | 49.532 | 1.00 | 20.00 |
| ATOM | 1241 | CE | LYS | 443 | 23.348 | 1.248 | 48.686 | 1.00 | 20.00 |
| ATOM | 1242 | NZ | LYS | 443 | 22.704 | 1.018 | 47.374 | 1.00 | 20.00 |
| ATOM | 1246 | C | LYS | 443 | 24.824 | -2.413 | 52.734 | 1.00 | 20.00 |
| ATOM | 1247 | O | LYS | 443 | 23.798 | -2.535 | 53.398 | 1.00 | 20.00 |
| ATOM | 1248 | N | ASN | 444 | 25.920 | -3.155 | 52.963 | 1.00 | 20.00 |
| ATOM | 1250 | CA | ASN | 444 | 26.027 | -4.165 | 53.984 | 1.00 | 20.00 |
| ATOM | 1251 | CB | ASN | 444 | 27.114 | -5.208 | 53.675 | 1.00 | 20.00 |
| ATOM | 1252 | CG | ASN | 444 | 26.577 | -6.095 | 52.559 | 1.00 | 20.00 |
| ATOM | 1253 | OD1 | ASN | 444 | 25.369 | -6.297 | 52.447 | 1.00 | 20.00 |
| ATOM | 1254 | ND2 | ASN | 444 | 27.490 | -6.648 | 51.717 | 1.00 | 20.00 |
| ATOM | 1257 | C | ASN | 444 | 26.247 | -3.673 | 55.387 | 1.00 | 20.00 |
| ATOM | 1258 | O | ASN | 444 | 26.107 | -4.446 | 56.333 | 1.00 | 20.00 |
| ATOM | 1259 | N | LEU | 445 | 26.670 | -2.409 | 55.575 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1261 | CA | LEU | 445 | 27.029 | -1.962 | 56.894 | 1.00 | 20.00 |
| ATOM | 1262 | CB | LEU | 445 | 27.608 | -0.533 | 56.890 | 1.00 | 20.00 |
| ATOM | 1263 | CG | LEU | 445 | 28.021 | -0.002 | 58.276 | 1.00 | 20.00 |
| DM | 1264 | CD1 | LEU | 445 | 29.207 | -0.798 | 58.846 | 1.00 | 20.00 |
| ATOM | 1265 | CD2 | LEU | 445 | 28.286 | 1.512 | 58.239 | 1.00 | 20.00 |
| ATOM | 1266 | C | LEU | 445 | 25.880 | -2.002 | 57.855 | 1.00 | 20.00 |
| ATOM | 1267 | O | LEU | 445 | 24.803 | -1.466 | 57.601 | 1.00 | 20.00 |
| ATOM | 1268 | N | CYS | 446 | 26.109 | -2.656 | 59.011 | 1.00 | 20.00 |
| ATOM | 1270 | CA | CYS | 446 | 25.129 | -2.767 | 60.051 | 1.00 | 20.00 |
| ATOM | 1271 | CB | CYS | 446 | 24.604 | -4.196 | 60.270 | 1.00 | 20.00 |
| ATOM | 1272 | SG | CYS | 446 | 23.521 | -4.750 | 58.922 | 1.00 | 20.00 |
| ATOM | 1273 | C | CYS | 446 | 25.815 | -2.339 | 61.305 | 1.00 | 20.00 |
| ATOM | 1274 | O | CYS | 446 | 26.913 | -1.790 | 61.261 | 1.00 | 20.00 |
| ATOM | 1275 | N | TYR | 447 | 25.170 | -2.551 | 62.467 | 1.00 | 20.00 |
| ATOM | 1277 | CA | TYR | 447 | 25.788 | -2.176 | 63.704 | 1.00 | 20.00 |
| ATOM | 1278 | CB | TYR | 447 | 27.139 | -2.860 | 63.933 | 1.00 | 20.00 |
| ATOM | 1279 | CG | TYR | 447 | 26.901 | -4.315 | 64.050 | 1.00 | 20.00 |
| ATOM | 1280 | CD1 | TYR | 447 | 26.684 | -5.079 | 62.926 | 1.00 | 20.00 |
| ATOM | 1281 | CE1 | TYR | 447 | 26.536 | -6.440 | 63.018 | 1.00 | 20.00 |
| ATOM | 1282 | CD2 | TYR | 447 | 27.005 | -4.920 | 65.274 | 1.00 | 20.00 |
| ATOM | 1283 | CE2 | TYR | 447 | 26.887 | -6.280 | 65.362 | 1.00 | 20.00 |
| ATOM | 1284 | CZ | TYR | 447 | 26.639 | -7.040 | 64.246 | 1.00 | 20.00 |
| ATOM | 1285 | OH | TYR | 447 | 26.509 | -8.439 | 64.357 | 1.00 | 20.00 |
| ATOM | 1287 | C | TYR | 447 | 26.099 | -0.718 | 63.647 | 1.00 | 20.00 |
| ATOM | 1288 | O | TYR | 447 | 27.098 | -0.285 | 64.220 | 1.00 | 20.00 |
| ATOM | 1289 | N | ALA | 448 | 25.354 | 0.035 | 62.816 | 1.00 | 20.00 |
| ATOM | 1291 | CA | ALA | 448 | 25.444 | 1.468 | 62.731 | 1.00 | 20.00 |
| ATOM | 1292 | CB | ALA | 448 | 25.053 | 1.995 | 61.341 | 1.00 | 20.00 |
| ATOM | 1293 | C | ALA | 448 | 24.577 | 2.186 | 63.723 | 1.00 | 20.00 |
| ATOM | 1294 | O | ALA | 448 | 24.983 | 3.172 | 64.335 | 1.00 | 20.00 |
| ATOM | 1295 | N | ASN | 449 | 23.326 | 1.702 | 63.860 | 1.00 | 20.00 |
| ATOM | 1297 | CA | ASN | 449 | 22.283 | 2.266 | 64.675 | 1.00 | 20.00 |
| ATOM | 1298 | CB | ASN | 449 | 20.909 | 1.646 | 64.371 | 1.00 | 20.00 |
| ATOM | 1299 | CG | ASN | 449 | 20.560 | 1.977 | 62.927 | 1.00 | 20.00 |
| ATOM | 1300 | OD1 | ASN | 449 | 20.287 | 1.088 | 62.122 | 1.00 | 20.00 |
| ATOM | 1301 | ND2 | ASN | 449 | 20.574 | 3.293 | 62.586 | 1.00 | 20.00 |
| ATOM | 1304 | C | ASN | 449 | 22.569 | 2.021 | 66.116 | 1.00 | 20.00 |
| ATOM | 1305 | O | ASN | 449 | 22.047 | 2.695 | 67.001 | 1.00 | 20.00 |
| ATOM | 1306 | N | THR | 450 | 23.375 | 0.983 | 66.361 | 1.00 | 20.00 |
| ATOM | 1308 | CA | THR | 450 | 23.740 | 0.473 | 67.644 | 1.00 | 20.00 |
| ATOM | 1309 | CB | THR | 450 | 24.470 | -0.828 | 67.513 | 1.00 | 20.00 |
| ATOM | 1310 | OG1 | THR | 450 | 23.769 | -1.689 | 66.632 | 1.00 | 20.00 |
| ATOM | 1312 | CG2 | THR | 450 | 24.492 | -1.486 | 68.896 | 1.00 | 20.00 |
| ATOM | 1313 | C | THR | 450 | 24.647 | 1.405 | 68.395 | 1.00 | 20.00 |
| ATOM | 1314 | O | THR | 450 | 24.795 | 1.253 | 69.605 | 1.00 | 20.00 |
| ATOM | 1315 | N | ILE | 451 | 25.329 | 2.350 | 67.707 | 1.00 | 20.00 |
| ATOM | 1317 | CA | ILE | 451 | 26.316 | 3.163 | 68.373 | 1.00 | 20.00 |
| ATOM | 1318 | CB | ILE | 451 | 27.580 | 3.277 | 67.555 | 1.00 | 20.00 |
| ATOM | 1319 | CG2 | ILE | 451 | 27.299 | 4.270 | 66.414 | 1.00 | 20.00 |
| ATOM | 1320 | CG1 | ILE | 451 | 28.815 | 3.653 | 68.399 | 1.00 | 20.00 |
| ATOM | 1321 | CD1 | ILE | 451 | 28.834 | 5.086 | 68.923 | 1.00 | 20.00 |
| ATOM | 1322 | C | ILE | 451 | 25.818 | 4.546 | 68.693 | 1.00 | 20.00 |
| ATOM | 1323 | O | ILE | 451 | 25.096 | 5.166 | 67.913 | 1.00 | 20.00 |
| ATOM | 1324 | N | ASN | 452 | 26.191 | 5.056 | 69.889 | 1.00 | 20.00 |
| ATOM | 1326 | CA | ASN | 452 | 25.793 | 6.369 | 70.309 | 1.00 | 20.00 |
| ATOM | 1327 | CB | ASN | 452 | 25.558 | 6.442 | 71.830 | 1.00 | 20.00 |
| ATOM | 1328 | CG | ASN | 452 | 24.657 | 7.627 | 72.151 | 1.00 | 20.00 |
| ATOM | 1329 | OD1 | ASN | 452 | 24.663 | 8.643 | 71.460 | 1.00 | 20.00 |
| ATOM | 1330 | ND2 | ASN | 452 | 23.848 | 7.489 | 73.236 | 1.00 | 20.00 |
| ATOM | 1333 | C | ASN | 452 | 26.916 | 7.303 | 69.951 | 1.00 | 20.00 |
| ATOM | 1334 | O | ASN | 452 | 27.858 | 7.507 | 70.716 | 1.00 | 20.00 |
| ATOM | 1335 | N | TRP | 453 | 26.809 | 7.922 | 68.762 | 1.00 | 20.00 |
| ATOM | 1337 | CA | TRP | 453 | 27.799 | 8.801 | 68.207 | 1.00 | 20.00 |
| ATOM | 1338 | CB | TRP | 453 | 27.480 | 9.218 | 66.759 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1339 | CG | TRP | 453 | 27.480 | 8.071 | 65.773 | 1.00 | 20.00 |
| ATOM | 1340 | CD2 | TRP | 453 | 28.653 | 7.348 | 65.358 | 1.00 | 20.00 |
| ATOM | 1341 | CE2 | TRP | 453 | 28.237 | 6.354 | 64.473 | 1.00 | 20.00 |
| ATOM | 1342 | CE3 | TRP | 453 | 29.967 | 7.498 | 65.690 | 1.00 | 20.00 |
| ATOM | 1343 | CD1 | TRP | 453 | 26.422 | 7.468 | 65.152 | 1.00 | 20.00 |
| ATOM | 1344 | NE1 | TRP | 453 | 26.867 | 6.442 | 64.354 | 1.00 | 20.00 |
| ATOM | 1346 | CZ2 | TRP | 453 | 29.138 | 5.503 | 63.898 | 1.00 | 20.00 |
| ATOM | 1347 | CZ3 | TRP | 453 | 30.876 | 6.651 | 65.095 | 1.00 | 20.00 |
| ATOM | 1348 | CH2 | TRP | 453 | 30.468 | 5.670 | 64.215 | 1.00 | 20.00 |
| ATOM | 1349 | C | TRP | 453 | 27.873 | 10.031 | 69.043 | 1.00 | 20.00 |
| ATOM | 1350 | O | TRP | 453 | 28.849 | 10.771 | 68.982 | 1.00 | 20.00 |
| ATOM | 1351 | N | LYS | 454 | 26.814 | 10.303 | 69.823 | 1.00 | 20.00 |
| ATOM | 1353 | CA | LYS | 454 | 26.774 | 11.481 | 70.637 | 1.00 | 20.00 |
| ATOM | 1354 | CB | LYS | 454 | 25.501 | 11.532 | 71.502 | 1.00 | 20.00 |
| ATOM | 1355 | CG | LYS | 454 | 25.282 | 12.849 | 72.250 | 1.00 | 20.00 |
| ATOM | 1356 | CD | LYS | 454 | 23.876 | 12.981 | 72.840 | 1.00 | 20.00 |
| ATOM | 1357 | CE | LYS | 454 | 23.801 | 12.650 | 74.332 | 1.00 | 20.00 |
| ATOM | 1358 | NZ | LYS | 454 | 24.177 | 11.237 | 74.560 | 1.00 | 20.00 |
| ATOM | 1362 | C | LYS | 454 | 27.947 | 11.473 | 71.563 | 1.00 | 20.00 |
| ATOM | 1363 | O | LYS | 454 | 28.592 | 12.501 | 71.763 | 1.00 | 20.00 |
| ATOM | 1364 | N | LYS | 455 | 28.249 | 10.309 | 72.167 | 1.00 | 20.00 |
| ATOM | 1366 | CA | LYS | 455 | 29.358 | 10.234 | 73.073 | 1.00 | 20.00 |
| ATOM | 1367 | CB | LYS | 455 | 29.457 | 8.875 | 73.785 | 1.00 | 20.00 |
| ATOM | 1368 | CG | LYS | 455 | 30.614 | 8.799 | 74.783 | 1.00 | 20.00 |
| ATOM | 1369 | CD | LYS | 455 | 30.517 | 7.613 | 75.745 | 1.00 | 20.00 |
| ATOM | 1370 | CE | LYS | 455 | 31.670 | 7.543 | 76.748 | 1.00 | 20.00 |
| ATOM | 1371 | NZ | LYS | 455 | 31.474 | 6.401 | 77.669 | 1.00 | 20.00 |
| ATOM | 1375 | C | LYS | 455 | 30.646 | 10.448 | 72.341 | 1.00 | 20.00 |
| ATOM | 1376 | O | LYS | 455 | 31.520 | 11.181 | 72.801 | 1.00 | 20.00 |
| ATOM | 1377 | N | LEU | 456 | 30.793 | 9.802 | 71.171 | 1.00 | 20.00 |
| ATOM | 1379 | CA | LEU | 456 | 32.005 | 9.890 | 70.405 | 1.00 | 20.00 |
| ATOM | 1380 | CB | LEU | 456 | 31.950 | 8.928 | 69.195 | 1.00 | 20.00 |
| ATOM | 1381 | CG | LEU | 456 | 33.236 | 8.741 | 68.352 | 1.00 | 20.00 |
| ATOM | 1382 | CD1 | LEU | 456 | 32.974 | 7.740 | 67.215 | 1.00 | 20.00 |
| ATOM | 1383 | CD2 | LEU | 456 | 33.819 | 10.056 | 67.809 | 1.00 | 20.00 |
| ATOM | 1384 | C | LEU | 456 | 32.207 | 11.296 | 69.921 | 1.00 | 20.00 |
| ATOM | 1385 | O | LEU | 456 | 33.299 | 11.850 | 70.051 | 1.00 | 20.00 |
| ATOM | 1386 | N | PHE | 457 | 31.152 | 11.919 | 69.356 | 1.00 | 20.00 |
| ATOM | 1388 | CA | PHE | 457 | 31.275 | 13.239 | 68.804 | 1.00 | 20.00 |
| ATOM | 1389 | CB | PHE | 457 | 30.520 | 13.432 | 67.483 | 1.00 | 20.00 |
| ATOM | 1390 | CG | PHE | 457 | 31.040 | 12.438 | 66.521 | 1.00 | 20.00 |
| ATOM | 1391 | CD1 | PHE | 457 | 32.171 | 12.700 | 65.787 | 1.00 | 20.00 |
| ATOM | 1392 | CD2 | PHE | 457 | 30.393 | 11.236 | 66.379 | 1.00 | 20.00 |
| ATOM | 1393 | CE1 | PHE | 457 | 32.660 | 11.752 | 64.926 | 1.00 | 20.00 |
| ATOM | 1394 | CE2 | PHE | 457 | 30.882 | 10.287 | 65.522 | 1.00 | 20.00 |
| ATOM | 1395 | CZ | PHE | 457 | 32.031 | 10.535 | 64.819 | 1.00 | 20.00 |
| ATOM | 1396 | C | PHE | 457 | 30.582 | 14.189 | 69.714 | 1.00 | 20.00 |
| ATOM | 1397 | O | PHE | 457 | 29.355 | 14.198 | 69.791 | 1.00 | 20.00 |
| ATOM | 1398 | N | GLY | 458 | 31.351 | 14.991 | 70.462 | 1.00 | 40.00 |
| ATOM | 1400 | CA | GLY | 458 | 30.716 | 15.995 | 71.255 | 1.00 | 40.00 |
| ATOM | 1401 | C | GLY | 458 | 30.329 | 17.121 | 70.356 | 1.00 | 40.00 |
| ATOM | 1402 | O | GLY | 458 | 29.233 | 17.673 | 70.446 | 1.00 | 40.00 |
| ATOM | 1403 | N | THR | 459 | 31.242 | 17.448 | 69.423 | 1.00 | 40.00 |
| ATOM | 1405 | CA | THR | 459 | 31.117 | 18.607 | 68.594 | 1.00 | 40.00 |
| ATOM | 1406 | CB | THR | 459 | 32.178 | 18.671 | 67.530 | 1.00 | 40.00 |
| ATOM | 1407 | OG1 | THR | 459 | 32.074 | 17.559 | 66.653 | 1.00 | 40.00 |
| ATOM | 1409 | CG2 | THR | 459 | 33.557 | 18.683 | 68.213 | 1.00 | 40.00 |
| ATOM | 1410 | C | THR | 459 | 29.793 | 18.691 | 67.916 | 1.00 | 40.00 |
| ATOM | 1411 | O | THR | 459 | 29.038 | 19.634 | 68.147 | 1.00 | 40.00 |
| ATOM | 1412 | N | SER | 460 | 29.448 | 17.707 | 67.070 | 1.00 | 40.00 |
| ATOM | 1414 | CA | SER | 460 | 28.205 | 17.880 | 66.388 | 1.00 | 40.00 |
| ATOM | 1415 | CB | SER | 460 | 28.307 | 18.854 | 65.203 | 1.00 | 40.00 |
| ATOM | 1416 | OG | SER | 460 | 27.047 | 18.984 | 64.566 | 1.00 | 40.00 |
| ATOM | 1418 | C | SER | 460 | 27.707 | 16.589 | 65.838 | 1.00 | 40.00 |

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| ATOM | 1419 | O | SER | 460 | 28.122 | 16.158 | 64.765 | 1.00 | 40.00 |
| ATOM | 1420 | N | GLY | 461 | 26.798 | 15.935 | 66.578 | 1.00 | 40.00 |
| ATOM | 1422 | CA | GLY | 461 | 26.202 | 14.721 | 66.113 | 1.00 | 40.00 |
| ATOM | 1423 | C | GLY | 461 | 25.299 | 15.063 | 64.973 | 1.00 | 40.00 |
| ATOM | 1424 | O | GLY | 461 | 25.091 | 14.265 | 64.062 | 1.00 | 40.00 |
| ATOM | 1425 | N | GLN | 462 | 24.725 | 16.279 | 65.013 | 1.00 | 40.00 |
| ATOM | 1427 | CA | GLN | 462 | 23.786 | 16.715 | 64.020 | 1.00 | 40.00 |
| ATOM | 1428 | CB | GLN | 462 | 23.223 | 18.115 | 64.315 | 1.00 | 40.00 |
| ATOM | 1429 | CG | GLN | 462 | 24.287 | 19.212 | 64.282 | 1.00 | 40.00 |
| ATOM | 1430 | CD | GLN | 462 | 23.621 | 20.547 | 64.584 | 1.00 | 40.00 |
| ATOM | 1431 | OE1 | GLN | 462 | 22.443 | 20.753 | 64.300 | 1.00 | 40.00 |
| ATOM | 1432 | NE2 | GLN | 462 | 24.401 | 21.484 | 65.187 | 1.00 | 40.00 |
| ATOM | 1435 | C | GLN | 462 | 24.444 | 16.755 | 62.677 | 1.00 | 40.00 |
| ATOM | 1436 | O | GLN | 462 | 23.805 | 16.489 | 61.660 | 1.00 | 40.00 |
| ATOM | 1437 | N | LYS | 463 | 25.746 | 17.092 | 62.649 | 1.00 | 40.00 |
| ATOM | 1439 | CA | LYS | 463 | 26.507 | 17.247 | 61.440 | 1.00 | 40.00 |
| ATOM | 1440 | CB | LYS | 463 | 27.923 | 17.786 | 61.702 | 1.00 | 40.00 |
| ATOM | 1441 | CG | LYS | 463 | 28.590 | 18.361 | 60.452 | 1.00 | 40.00 |
| ATOM | 1442 | CD | LYS | 463 | 27.908 | 19.641 | 59.963 | 1.00 | 40.00 |
| ATOM | 1443 | CE | LYS | 463 | 28.550 | 20.258 | 58.720 | 1.00 | 40.00 |
| ATOM | 1444 | NZ | LYS | 463 | 27.801 | 21.469 | 58.318 | 1.00 | 40.00 |
| ATOM | 1448 | C | LYS | 463 | 26.660 | 15.969 | 60.669 | 1.00 | 40.00 |
| ATOM | 1449 | O | LYS | 463 | 26.753 | 15.991 | 59.443 | 1.00 | 40.00 |
| ATOM | 1450 | N | THR | 464 | 26.712 | 14.816 | 61.359 | 1.00 | 40.00 |
| ATOM | 1452 | CA | THR | 464 | 26.955 | 13.574 | 60.676 | 1.00 | 40.00 |
| ATOM | 1453 | CB | THR | 464 | 26.867 | 12.373 | 61.572 | 1.00 | 40.00 |
| ATOM | 1454 | OG1 | THR | 464 | 27.293 | 11.210 | 60.877 | 1.00 | 40.00 |
| ATOM | 1456 | CG2 | THR | 464 | 25.409 | 12.209 | 62.037 | 1.00 | 40.00 |
| ATOM | 1457 | C | THR | 464 | 26.008 | 13.353 | 59.545 | 1.00 | 40.00 |
| ATOM | 1458 | O | THR | 464 | 24.823 | 13.670 | 59.636 | 1.00 | 40.00 |
| ATOM | 1459 | N | LYS | 465 | 26.533 | 12.820 | 58.419 | 1.00 | 40.00 |
| ATOM | 1461 | CA | LYS | 465 | 25.666 | 12.528 | 57.319 | 1.00 | 40.00 |
| ATOM | 1462 | CB | LYS | 465 | 26.015 | 13.230 | 55.998 | 1.00 | 40.00 |
| ATOM | 1463 | CG | LYS | 465 | 24.994 | 12.891 | 54.910 | 1.00 | 40.00 |
| ATOM | 1464 | CD | LYS | 465 | 25.020 | 13.816 | 53.693 | 1.00 | 40.00 |
| ATOM | 1465 | CE | LYS | 465 | 23.979 | 13.435 | 52.638 | 1.00 | 40.00 |
| ATOM | 1466 | NZ | LYS | 465 | 23.968 | 14.436 | 51.549 | 1.00 | 40.00 |
| ATOM | 1470 | C | LYS | 465 | 25.706 | 11.064 | 57.057 | 1.00 | 40.00 |
| ATOM | 1471 | O | LYS | 465 | 26.759 | 10.491 | 56.776 | 1.00 | 40.00 |
| ATOM | 1472 | N | ILE | 466 | 24.532 | 10.415 | 57.150 | 1.00 | 40.00 |
| ATOM | 1474 | CA | ILE | 466 | 24.500 | 9.007 | 56.923 | 1.00 | 40.00 |
| ATOM | 1475 | CB | ILE | 466 | 24.176 | 8.233 | 58.167 | 1.00 | 40.00 |
| ATOM | 1476 | CG2 | ILE | 466 | 24.064 | 6.747 | 57.789 | 1.00 | 40.00 |
| ATOM | 1477 | CG1 | ILE | 466 | 25.226 | 8.516 | 59.256 | 1.00 | 40.00 |
| ATOM | 1478 | CD1 | ILE | 466 | 24.825 | 8.003 | 60.639 | 1.00 | 40.00 |
| ATOM | 1479 | C | ILE | 466 | 23.436 | 8.713 | 55.920 | 1.00 | 40.00 |
| ATOM | 1480 | O | ILE | 466 | 22.278 | 9.088 | 56.102 | 1.00 | 40.00 |
| ATOM | 1481 | N | ILE | 467 | 23.821 | 8.046 | 54.814 | 1.00 | 40.00 |
| ATOM | 1483 | CA | ILE | 467 | 22.874 | 7.661 | 53.810 | 1.00 | 40.00 |
| ATOM | 1484 | CB | ILE | 467 | 22.588 | 8.736 | 52.798 | 1.00 | 40.00 |
| ATOM | 1485 | CG2 | ILE | 467 | 21.923 | 9.922 | 53.515 | 1.00 | 40.00 |
| ATOM | 1486 | CG1 | ILE | 467 | 23.865 | 9.111 | 52.030 | 1.00 | 40.00 |
| ATOM | 1487 | CD1 | ILE | 467 | 23.596 | 9.992 | 50.811 | 1.00 | 40.00 |
| ATOM | 1488 | C | ILE | 467 | 23.454 | 6.505 | 53.058 | 1.00 | 40.00 |
| ATOM | 1489 | O | ILE | 467 | 24.671 | 6.345 | 52.991 | 1.00 | 40.00 |
| ATOM | 1490 | N | SER | 468 | 22.575 | 5.682 | 52.452 | 1.00 | 40.00 |
| ATOM | 1492 | CA | SER | 468 | 22.961 | 4.556 | 51.646 | 1.00 | 40.00 |
| ATOM | 1493 | CB | SER | 468 | 24.002 | 4.934 | 50.577 | 1.00 | 40.00 |
| ATOM | 1494 | OG | SER | 468 | 23.458 | 5.896 | 49.686 | 1.00 | 40.00 |
| ATOM | 1496 | C | SER | 468 | 23.509 | 3.382 | 52.407 | 1.00 | 40.00 |
| ATOM | 1497 | O | SER | 468 | 24.142 | 2.512 | 51.810 | 1.00 | 40.00 |
| ATOM | 1498 | N | ASN | 469 | 23.263 | 3.292 | 53.729 | 1.00 | 20.00 |
| ATOM | 1500 | CA | ASN | 469 | 23.744 | 2.155 | 54.472 | 1.00 | 20.00 |
| ATOM | 1501 | CB | ASN | 469 | 24.112 | 2.474 | 55.930 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1502 | CG | ASN | 469 | 25.381 | 3.315 | 55.913 | 1.00 | 20.00 |
| ATOM | 1503 | OD1 | ASN | 469 | 26.339 | 3.005 | 55.205 | 1.00 | 20.00 |
| ATOM | 1504 | ND2 | ASN | 469 | 25.388 | 4.414 | 56.712 | 1.00 | 20.00 |
| ATOM | 1507 | C | ASN | 469 | 22.672 | 1.112 | 54.485 | 1.00 | 20.00 |
| ATOM | 1508 | O | ASN | 469 | 21.660 | 1.240 | 53.800 | 1.00 | 20.00 |
| ATOM | 1509 | N | ARG | 470 | 22.877 | 0.022 | 55.254 | 1.00 | 20.00 |
| ATOM | 1511 | CA | ARG | 470 | 21.898 | -1.026 | 55.268 | 1.00 | 20.00 |
| ATOM | 1512 | CB | ARG | 470 | 22.443 | -2.371 | 55.776 | 1.00 | 20.00 |
| ATOM | 1513 | CG | ARG | 470 | 21.540 | -3.550 | 55.415 | 1.00 | 20.00 |
| ATOM | 1514 | CD | ARG | 470 | 22.221 | -4.913 | 55.539 | 1.00 | 20.00 |
| ATOM | 1515 | NE | ARG | 470 | 21.220 | -5.939 | 55.132 | 1.00 | 20.00 |
| ATOM | 1517 | CZ | ARG | 470 | 21.018 | -6.201 | 53.807 | 1.00 | 20.00 |
| ATOM | 1518 | NH1 | ARG | 470 | 20.128 | -7.165 | 53.429 | 1.00 | 20.00 |
| ATOM | 1521 | NH2 | ARG | 470 | 21.699 | -5.492 | 52.859 | 1.00 | 20.00 |
| ATOM | 1524 | C | ARG | 470 | 20.742 | -0.619 | 56.128 | 1.00 | 20.00 |
| ATOM | 1525 | O | ARG | 470 | 20.889 | 0.183 | 57.048 | 1.00 | 20.00 |
| ATOM | 1526 | N | GLY | 471 | 19.546 | -1.171 | 55.835 | 1.00 | 20.00 |
| ATOM | 1528 | CA | GLY | 471 | 18.369 | -0.820 | 56.575 | 1.00 | 20.00 |
| ATOM | 1529 | C | GLY | 471 | 18.410 | -1.520 | 57.892 | 1.00 | 20.00 |
| ATOM | 1530 | O | GLY | 471 | 18.635 | -2.726 | 57.968 | 1.00 | 20.00 |
| ATOM | 1531 | N | GLU | 472 | 18.110 | -0.768 | 58.964 | 1.00 | 20.00 |
| ATOM | 1533 | CA | GLU | 472 | 18.175 | -1.258 | 60.308 | 1.00 | 20.00 |
| ATOM | 1534 | CB | GLU | 472 | 17.700 | -0.191 | 61.312 | 1.00 | 20.00 |
| ATOM | 1535 | CG | GLU | 472 | 17.766 | -0.618 | 62.778 | 1.00 | 20.00 |
| ATOM | 1536 | CD | GLU | 472 | 17.265 | 0.550 | 63.621 | 1.00 | 20.00 |
| ATOM | 1537 | OE1 | GLU | 472 | 17.843 | 1.662 | 63.488 | 1.00 | 20.00 |
| ATOM | 1538 | OE2 | GLU | 472 | 16.297 | 0.348 | 64.401 | 1.00 | 20.00 |
| ATOM | 1539 | C | GLU | 472 | 17.281 | -2.449 | 60.428 | 1.00 | 20.00 |
| ATOM | 1540 | O | GLU | 472 | 17.601 | -3.408 | 61.131 | 1.00 | 20.00 |
| ATOM | 1541 | N | ASN | 473 | 16.126 | -2.412 | 59.741 | 1.00 | 20.00 |
| ATOM | 1543 | CA | ASN | 473 | 15.193 | -3.499 | 59.794 | 1.00 | 20.00 |
| ATOM | 1544 | CB | ASN | 473 | 13.928 | -3.214 | 58.965 | 1.00 | 20.00 |
| ATOM | 1545 | CG | ASN | 473 | 13.138 | -2.118 | 59.669 | 1.00 | 20.00 |
| ATOM | 1546 | OD1 | ASN | 473 | 12.431 | -2.374 | 60.643 | 1.00 | 20.00 |
| ATOM | 1547 | ND2 | ASN | 473 | 13.264 | -0.859 | 59.169 | 1.00 | 20.00 |
| ATOM | 1550 | C | ASN | 473 | 15.837 | -4.727 | 59.232 | 1.00 | 20.00 |
| ATOM | 1551 | O | ASN | 473 | 15.707 | -5.817 | 59.788 | 1.00 | 20.00 |
| ATOM | 1552 | N | SER | 474 | 16.555 | -4.573 | 58.103 | 1.00 | 20.00 |
| ATOM | 1554 | CA | SER | 474 | 17.194 | -5.681 | 57.451 | 1.00 | 20.00 |
| ATOM | 1555 | CB | SER | 474 | 17.843 | -5.283 | 56.113 | 1.00 | 20.00 |
| ATOM | 1556 | OG | SER | 474 | 18.457 | -6.413 | 55.510 | 1.00 | 20.00 |
| ATOM | 1558 | C | SER | 474 | 18.276 | -6.232 | 58.324 | 1.00 | 20.00 |
| ATOM | 1559 | O | SER | 474 | 18.449 | -7.445 | 58.429 | 1.00 | 20.00 |
| ATOM | 1560 | N | CYS | 475 | 19.036 | -5.344 | 58.987 | 1.00 | 20.00 |
| ATOM | 1562 | CA | CYS | 475 | 20.125 | -5.779 | 59.808 | 1.00 | 20.00 |
| ATOM | 1563 | CB | CYS | 475 | 20.906 | -4.613 | 60.438 | 1.00 | 20.00 |
| ATOM | 1564 | SG | CYS | 475 | 21.836 | -3.652 | 59.208 | 1.00 | 20.00 |
| ATOM | 1565 | C | CYS | 475 | 19.582 | -6.621 | 60.912 | 1.00 | 20.00 |
| ATOM | 1566 | O | CYS | 475 | 20.186 | -7.628 | 61.278 | 1.00 | 20.00 |
| ATOM | 1567 | N | LYS | 476 | 18.409 | -6.242 | 61.459 | 1.00 | 60.00 |
| ATOM | 1569 | CA | LYS | 476 | 17.874 | -6.990 | 62.558 | 1.00 | 60.00 |
| ATOM | 1570 | CB | LYS | 476 | 17.613 | -8.468 | 62.216 | 1.00 | 60.00 |
| ATOM | 1571 | CG | LYS | 476 | 16.317 | -8.703 | 61.436 | 1.00 | 60.00 |
| ATOM | 1572 | CD | LYS | 476 | 15.048 | -8.476 | 62.266 | 1.00 | 60.00 |
| ATOM | 1573 | CE | LYS | 476 | 14.947 | -7.089 | 62.904 | 1.00 | 60.00 |
| ATOM | 1574 | NZ | LYS | 476 | 13.748 | -7.017 | 63.770 | 1.00 | 60.00 |
| ATOM | 1578 | C | LYS | 476 | 18.921 | -6.920 | 63.604 | 1.00 | 60.00 |
| ATOM | 1579 | O | LYS | 476 | 19.139 | -7.855 | 64.372 | 1.00 | 60.00 |
| ATOM | 1580 | N | ALA | 477 | 19.596 | -5.764 | 63.640 | 1.00 | 60.00 |
| ATOM | 1582 | CA | ALA | 477 | 20.675 | -5.551 | 64.538 | 1.00 | 60.00 |
| ATOM | 1583 | CB | ALA | 477 | 21.779 | -4.658 | 63.931 | 1.00 | 60.00 |
| ATOM | 1584 | C | ALA | 477 | 20.208 | -4.882 | 65.785 | 1.00 | 60.00 |
| ATOM | 1585 | O | ALA | 477 | 19.038 | -4.543 | 65.960 | 1.00 | 60.00 |
| ATOM | 1586 | N | THR | 478 | 21.182 | -4.797 | 66.700 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1588 | CA | THR | 478 | 21.298 | -4.164 | 67.976 | 1.00 | 60.00 |
| ATOM | 1589 | CB | THR | 478 | 20.348 | -4.676 | 69.025 | 1.00 | 60.00 |
| ATOM | 1590 | OG1 | THR | 478 | 20.460 | -6.086 | 69.145 | 1.00 | 60.00 |
| ATOM | 1592 | CG2 | THR | 478 | 18.907 | -4.266 | 68.681 | 1.00 | 60.00 |
| ATOM | 1593 | C | THR | 478 | 22.621 | -4.786 | 68.220 | 1.00 | 60.00 |
| ATOM | 1594 | O | THR | 478 | 22.914 | -5.304 | 69.294 | 1.00 | 60.00 |
| ATOM | 1595 | N | GLY | 479 | 23.468 | -4.695 | 67.178 | 1.00 | 60.00 |
| ATOM | 1597 | CA | GLY | 479 | 24.658 | -5.480 | 67.102 | 1.00 | 60.00 |
| ATOM | 1598 | C | GLY | 479 | 24.076 | -6.585 | 66.277 | 1.00 | 60.00 |
| ATOM | 1599 | O | GLY | 479 | 23.056 | -6.365 | 65.632 | 1.00 | 60.00 |
| ATOM | 1600 | N | GLN | 480 | 24.678 | -7.792 | 66.239 | 1.00 | 60.00 |
| ATOM | 1602 | CA | GLN | 480 | 23.982 | -8.847 | 65.552 | 1.00 | 60.00 |
| ATOM | 1603 | CB | GLN | 480 | 24.733 | -10.188 | 65.586 | 1.00 | 60.00 |
| ATOM | 1604 | CG | GLN | 480 | 24.025 | -11.318 | 64.839 | 1.00 | 60.00 |
| ATOM | 1605 | CD | GLN | 480 | 24.929 | -12.541 | 64.896 | 1.00 | 60.00 |
| ATOM | 1606 | OE1 | GLN | 480 | 24.989 | -13.330 | 63.955 | 1.00 | 60.00 |
| ATOM | 1607 | NE2 | GLN | 480 | 25.659 | -12.704 | 66.032 | 1.00 | 60.00 |
| ATOM | 1610 | C | GLN | 480 | 22.824 | -8.945 | 66.475 | 1.00 | 60.00 |
| ATOM | 1611 | O | GLN | 480 | 21.664 | -9.097 | 66.095 | 1.00 | 60.00 |
| ATOM | 1612 | N | VAL | 481 | 23.201 | -8.820 | 67.750 | 1.00 | 60.00 |
| ATOM | 1614 | CA | VAL | 481 | 22.411 | -8.694 | 68.923 | 1.00 | 60.00 |
| ATOM | 1615 | CB | VAL | 481 | 21.982 | -10.002 | 69.518 | 1.00 | 60.00 |
| ATOM | 1616 | CG1 | VAL | 481 | 23.239 | -10.779 | 69.947 | 1.00 | 60.00 |
| ATOM | 1617 | CG2 | VAL | 481 | 21.013 | -9.716 | 70.677 | 1.00 | 60.00 |
| ATOM | 1618 | C | VAL | 481 | 23.529 | -8.182 | 69.755 | 1.00 | 60.00 |
| ATOM | 1619 | O | VAL | 481 | 24.685 | -8.456 | 69.436 | 1.00 | 60.00 |
| ATOM | 1620 | N | CYS | 482 | 23.285 | -7.401 | 70.814 | 1.00 | 20.00 |
| ATOM | 1622 | CA | CYS | 482 | 24.503 | -7.039 | 71.462 | 1.00 | 20.00 |
| ATOM | 1623 | CB | CYS | 482 | 24.576 | -5.617 | 72.037 | 1.00 | 20.00 |
| ATOM | 1624 | SG | CYS | 482 | 26.326 | -5.221 | 72.294 | 1.00 | 20.00 |
| ATOM | 1625 | C | CYS | 482 | 24.696 | -8.015 | 72.582 | 1.00 | 20.00 |
| ATOM | 1626 | O | CYS | 482 | 23.907 | -8.945 | 72.738 | 1.00 | 20.00 |
| ATOM | 1627 | N | HIS | 483 | 25.765 | -7.848 | 73.388 | 1.00 | 20.00 |
| ATOM | 1629 | CA | HIS | 483 | 25.982 | -8.790 | 74.444 | 1.00 | 20.00 |
| ATOM | 1630 | CB | HIS | 483 | 27.387 | -8.739 | 75.065 | 1.00 | 20.00 |
| ATOM | 1631 | CG | HIS | 483 | 27.708 | -10.003 | 75.804 | 1.00 | 20.00 |
| ATOM | 1632 | CD2 | HIS | 483 | 28.282 | -11.158 | 75.361 | 1.00 | 20.00 |
| ATOM | 1633 | ND1 | HIS | 483 | 27.377 | -10.228 | 77.118 | 1.00 | 20.00 |
| ATOM | 1635 | CE1 | HIS | 483 | 27.769 | -11.494 | 77.410 | 1.00 | 20.00 |
| ATOM | 1636 | NE2 | HIS | 483 | 28.323 | -12.098 | 76.375 | 1.00 | 20.00 |
| ATOM | 1638 | C | HIS | 483 | 24.956 | -8.511 | 75.490 | 1.00 | 20.00 |
| ATOM | 1639 | O | HIS | 483 | 24.359 | -7.436 | 75.521 | 1.00 | 20.00 |
| ATOM | 1640 | N | ALA | 484 | 24.706 | -9.497 | 76.368 | 1.00 | 20.00 |
| ATOM | 1642 | CA | ALA | 484 | 23.706 | -9.332 | 77.379 | 1.00 | 20.00 |
| ATOM | 1643 | CB | ALA | 484 | 23.553 | -10.571 | 78.276 | 1.00 | 20.00 |
| ATOM | 1644 | C | ALA | 484 | 24.123 | -8.198 | 78.258 | 1.00 | 20.00 |
| ATOM | 1645 | O | ALA | 484 | 23.301 | -7.383 | 78.673 | 1.00 | 20.00 |
| ATOM | 1646 | N | LEU | 485 | 25.432 | -8.123 | 78.554 | 1.00 | 20.00 |
| ATOM | 1648 | CA | LEU | 485 | 25.971 | -7.130 | 79.435 | 1.00 | 20.00 |
| ATOM | 1649 | CB | LEU | 485 | 27.458 | -7.364 | 79.760 | 1.00 | 20.00 |
| ATOM | 1650 | CG | LEU | 485 | 27.723 | -8.604 | 80.636 | 1.00 | 20.00 |
| ATOM | 1651 | CD1 | LEU | 485 | 27.110 | -8.438 | 82.033 | 1.00 | 20.00 |
| ATOM | 1652 | CD2 | LEU | 485 | 27.254 | -9.899 | 79.959 | 1.00 | 20.00 |
| ATOM | 1653 | C | LEU | 485 | 25.859 | -5.731 | 78.922 | 1.00 | 20.00 |
| ATOM | 1654 | O | LEU | 485 | 25.609 | -4.816 | 79.705 | 1.00 | 20.00 |
| ATOM | 1655 | N | CYS | 486 | 26.059 | -5.521 | 77.605 | 1.00 | 20.00 |
| ATOM | 1657 | CA | CYS | 486 | 26.024 | -4.183 | 77.088 | 1.00 | 20.00 |
| ATOM | 1658 | CB | CYS | 486 | 26.159 | -4.089 | 75.561 | 1.00 | 20.00 |
| ATOM | 1659 | SG | CYS | 486 | 27.793 | -4.607 | 74.972 | 1.00 | 20.00 |
| ATOM | 1660 | C | CYS | 486 | 24.710 | -3.584 | 77.445 | 1.00 | 20.00 |
| ATOM | 1661 | O | CYS | 486 | 23.680 | -4.253 | 77.418 | 1.00 | 20.00 |
| ATOM | 1662 | N | SER | 487 | 24.725 | -2.298 | 77.834 | 1.00 | 40.00 |
| ATOM | 1664 | CA | SER | 487 | 23.489 | -1.683 | 78.191 | 1.00 | 40.00 |
| ATOM | 1665 | CB | SER | 487 | 23.641 | -0.401 | 79.021 | 1.00 | 40.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1666 | OG | SER | 487 | 24.221 | 0.618 | 78.222 | 1.00 | 40.00 |
| ATOM | 1668 | C | SER | 487 | 22.857 | -1.321 | 76.902 | 1.00 | 40.00 |
| ATOM | 1669 | O | SER | 487 | 23.476 | -1.424 | 75.845 | 1.00 | 40.00 |
| ATOM | 1670 | N | PRO | 488 | 21.639 | -0.873 | 76.994 | 1.00 | 40.00 |
| ATOM | 1671 | CD | PRO | 488 | 20.819 | -1.107 | 78.169 | 1.00 | 40.00 |
| ATOM | 1672 | CA | PRO | 488 | 20.856 | -0.523 | 75.848 | 1.00 | 40.00 |
| ATOM | 1673 | CB | PRO | 488 | 19.425 | -0.323 | 76.356 | 1.00 | 40.00 |
| ATOM | 1674 | CG | PRO | 488 | 19.548 | -0.293 | 77.891 | 1.00 | 40.00 |
| ATOM | 1675 | C | PRO | 488 | 21.442 | 0.669 | 75.183 | 1.00 | 40.00 |
| ATOM | 1676 | O | PRO | 488 | 20.909 | 1.090 | 74.158 | 1.00 | 40.00 |
| ATOM | 1677 | N | GLU | 489 | 22.526 | 1.231 | 75.750 | 1.00 | 40.00 |
| ATOM | 1679 | CA | GLU | 489 | 23.141 | 2.350 | 75.112 | 1.00 | 40.00 |
| ATOM | 1680 | CB | GLU | 489 | 24.424 | 2.824 | 75.815 | 1.00 | 40.00 |
| ATOM | 1681 | CG | GLU | 489 | 24.146 | 3.512 | 77.152 | 1.00 | 40.00 |
| ATOM | 1682 | CD | GLU | 489 | 23.356 | 4.780 | 76.856 | 1.00 | 40.00 |
| ATOM | 1683 | OE1 | GLU | 489 | 22.242 | 4.929 | 77.426 | 1.00 | 40.00 |
| ATOM | 1684 | OE2 | GLU | 489 | 23.854 | 5.615 | 76.055 | 1.00 | 40.00 |
| ATOM | 1685 | C | GLU | 489 | 23.486 | 1.912 | 73.726 | 1.00 | 40.00 |
| ATOM | 1686 | O | GLU | 489 | 23.147 | 2.591 | 72.758 | 1.00 | 40.00 |
| ATOM | 1687 | N | GLY | 490 | 24.148 | 0.746 | 73.581 | 1.00 | 40.00 |
| ATOM | 1689 | CA | GLY | 490 | 24.436 | 0.300 | 72.246 | 1.00 | 40.00 |
| ATOM | 1690 | C | GLY | 490 | 25.782 | -0.344 | 72.202 | 1.00 | 40.00 |
| ATOM | 1691 | O | GLY | 490 | 26.427 | -0.520 | 73.233 | 1.00 | 40.00 |
| ATOM | 1692 | N | CYS | 491 | 26.229 | -0.748 | 70.993 | 1.00 | 20.00 |
| ATOM | 1694 | CA | CYS | 491 | 27.534 | -1.322 | 70.876 | 1.00 | 20.00 |
| ATOM | 1695 | CB | CYS | 491 | 27.666 | -2.693 | 71.547 | 1.00 | 20.00 |
| ATOM | 1696 | SG | CYS | 491 | 26.822 | -4.060 | 70.710 | 1.00 | 20.00 |
| ATOM | 1697 | C | CYS | 491 | 27.974 | -1.427 | 69.448 | 1.00 | 20.00 |
| ATOM | 1698 | O | CYS | 491 | 27.191 | -1.256 | 68.516 | 1.00 | 20.00 |
| ATOM | 1699 | N | TRP | 492 | 29.286 | -1.658 | 69.249 | 1.00 | 20.00 |
| ATOM | 1701 | CA | TRP | 492 | 29.852 | -1.751 | 67.932 | 1.00 | 20.00 |
| ATOM | 1702 | CB | TRP | 492 | 31.383 | -1.624 | 67.949 | 1.00 | 20.00 |
| ATOM | 1703 | CG | TRP | 492 | 31.841 | -0.264 | 68.422 | 1.00 | 20.00 |
| ATOM | 1704 | CD2 | TRP | 492 | 31.829 | 0.923 | 67.613 | 1.00 | 20.00 |
| ATOM | 1705 | CE2 | TRP | 492 | 32.262 | 1.975 | 68.421 | 1.00 | 20.00 |
| ATOM | 1706 | CE3 | TRP | 492 | 31.478 | 1.122 | 66.309 | 1.00 | 20.00 |
| ATOM | 1707 | CD1 | TRP | 492 | 32.250 | 0.120 | 69.665 | 1.00 | 20.00 |
| ATOM | 1708 | NE1 | TRP | 492 | 32.522 | 1.466 | 69.675 | 1.00 | 20.00 |
| ATOM | 1710 | CZ2 | TRP | 492 | 32.349 | 3.248 | 67.934 | 1.00 | 20.00 |
| ATOM | 1711 | CZ3 | TRP | 492 | 31.572 | 2.407 | 65.820 | 1.00 | 20.00 |
| ATOM | 1712 | CH2 | TRP | 492 | 31.998 | 3.449 | 66.617 | 1.00 | 20.00 |
| ATOM | 1713 | C | TRP | 492 | 29.484 | -3.013 | 67.207 | 1.00 | 20.00 |
| ATOM | 1714 | O | TRP | 492 | 29.238 | -2.994 | 66.001 | 1.00 | 20.00 |
| ATOM | 1715 | N | GLY | 493 | 29.448 | -4.151 | 67.926 | 1.00 | 20.00 |
| ATOM | 1717 | CA | GLY | 493 | 29.135 | -5.416 | 67.316 | 1.00 | 20.00 |
| ATOM | 1718 | C | GLY | 493 | 28.919 | -6.347 | 68.463 | 1.00 | 20.00 |
| ATOM | 1719 | O | GLY | 493 | 28.646 | -5.883 | 69.565 | 1.00 | 20.00 |
| ATOM | 1720 | N | PRO | 494 | 28.961 | -7.638 | 68.284 | 1.00 | 40.00 |
| ATOM | 1721 | CD | PRO | 494 | 28.323 | -8.259 | 67.136 | 1.00 | 40.00 |
| ATOM | 1722 | CA | PRO | 494 | 28.822 | -8.443 | 69.463 | 1.00 | 40.00 |
| ATOM | 1723 | CB | PRO | 494 | 28.300 | -9.802 | 69.006 | 1.00 | 40.00 |
| ATOM | 1724 | CG | PRO | 494 | 27.573 | -9.482 | 67.689 | 1.00 | 40.00 |
| ATOM | 1725 | C | PRO | 494 | 30.128 | -8.514 | 70.185 | 1.00 | 40.00 |
| ATOM | 1726 | O | PRO | 494 | 31.072 | -9.053 | 69.613 | 1.00 | 40.00 |
| ATOM | 1727 | N | GLU | 495 | 30.195 | -8.014 | 71.436 | 1.00 | 40.00 |
| ATOM | 1729 | CA | GLU | 495 | 31.375 | -8.089 | 72.256 | 1.00 | 40.00 |
| ATOM | 1730 | CB | GLU | 495 | 32.593 | -7.287 | 71.749 | 1.00 | 40.00 |
| ATOM | 1731 | CG | GLU | 495 | 33.353 | -7.900 | 70.573 | 1.00 | 40.00 |
| ATOM | 1732 | CD | GLU | 495 | 34.454 | -6.930 | 70.171 | 1.00 | 40.00 |
| ATOM | 1733 | OE1 | GLU | 495 | 35.343 | -7.337 | 69.376 | 1.00 | 40.00 |
| ATOM | 1734 | OE2 | GLU | 495 | 34.417 | -5.764 | 70.646 | 1.00 | 40.00 |
| ATOM | 1735 | C | GLU | 495 | 31.004 | -7.432 | 73.546 | 1.00 | 40.00 |
| ATOM | 1736 | O | GLU | 495 | 30.221 | -6.486 | 73.553 | 1.00 | 40.00 |
| ATOM | 1737 | N | PRO | 496 | 31.509 | -7.915 | 74.645 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1738 | CD | PRO | 496 | 31.711 | -9.341 | 74.819 | 1.00 | 20.00 |
| ATOM | 1739 | CA | PRO | 496 | 31.264 | -7.251 | 75.897 | 1.00 | 20.00 |
| ATOM | 1740 | CB | PRO | 496 | 31.515 | -8.293 | 76.991 | 1.00 | 20.00 |
| i 4 | 1741 | CG | PRO | 496 | 32.200 | -9.467 | 76.268 | 1.00 | 20.00 |
| ATOM | 1742 | C | PRO | 496 | 32.127 | -6.031 | 76.014 | 1.00 | 20.00 |
| ATOM | 1743 | O | PRO | 496 | 31.852 | -5.174 | 76.853 | 1.00 | 20.00 |
| ATOM | 1744 | N | ARG | 497 | 33.221 | -5.983 | 75.231 | 1.00 | 20.00 |
| ATOM | 1746 | CA | ARG | 497 | 34.147 | -4.887 | 75.215 | 1.00 | 20.00 |
| ATOM | 1747 | CB | ARG | 497 | 35.506 | -5.301 | 74.623 | 1.00 | 20.00 |
| ATOM | 1748 | CG | ARG | 497 | 35.420 | -5.828 | 73.193 | 1.00 | 20.00 |
| ATOM | 1749 | CD | ARG | 497 | 36.661 | -6.603 | 72.744 | 1.00 | 20.00 |
| ATOM | 1750 | NE | ARG | 497 | 36.424 | -8.046 | 73.041 | 1.00 | 20.00 |
| ATOM | 1752 | CZ | ARG | 497 | 36.759 | -8.573 | 74.256 | 1.00 | 20.00 |
| ATOM | 1753 | NH1 | ARG | 497 | 37.298 | -7.778 | 75.225 | 1.00 | 20.00 |
| ATOM | 1756 | NH2 | ARG | 497 | 36.552 | -9.900 | 74.501 | 1.00 | 20.00 |
| ATOM | 1759 | C | ARG | 497 | 33.629 | -3.696 | 74.461 | 1.00 | 20.00 |
| ATOM | 1760 | O | ARG | 497 | 33.927 | -2.551 | 74.796 | 1.00 | 20.00 |
| ATOM | 1761 | N | ASP | 498 | 32.856 | -3.946 | 73.391 | 1.00 | 20.00 |
| ATOM | 1763 | CA | ASP | 498 | 32.360 | -2.918 | 72.516 | 1.00 | 20.00 |
| ATOM | 1764 | CB | ASP | 498 | 31.966 | -3.444 | 71.128 | 1.00 | 20.00 |
| ATOM | 1765 | CG | ASP | 498 | 30.893 | -4.496 | 71.291 | 1.00 | 20.00 |
| ATOM | 1766 | OD1 | ASP | 498 | 30.029 | -4.348 | 72.195 | 1.00 | 20.00 |
| ATOM | 1767 | OD2 | ASP | 498 | 30.949 | -5.482 | 70.511 | 1.00 | 20.00 |
| ATOM | 1768 | C | ASP | 498 | 31.265 | -2.044 | 73.055 | 1.00 | 20.00 |
| ATOM | 1769 | O | ASP | 498 | 31.035 | -0.965 | 72.509 | 1.00 | 20.00 |
| ATOM | 1770 | N | CYS | 499 | 30.544 | -2.499 | 74.102 | 1.00 | 20.00 |
| ATOM | 1772 | CA | CYS | 499 | 29.422 | -1.807 | 74.694 | 1.00 | 20.00 |
| ATOM | 1773 | CB | CYS | 499 | 29.165 | -2.202 | 76.162 | 1.00 | 20.00 |
| ATOM | 1774 | SG | CYS | 499 | 29.015 | -3.986 | 76.458 | 1.00 | 20.00 |
| ATOM | 1775 | C | CYS | 499 | 29.589 | -0.312 | 74.732 | 1.00 | 20.00 |
| ATOM | 1776 | O | CYS | 499 | 30.701 | 0.208 | 74.795 | 1.00 | 20.00 |
| ATOM | 1777 | N | VAL | 500 | 28.468 | 0.426 | 74.575 | 1.00 | 20.00 |
| ATOM | 1779 | CA | VAL | 500 | 28.473 | 1.851 | 74.753 | 1.00 | 20.00 |
| ATOM | 1780 | CB | VAL | 500 | 27.278 | 2.529 | 74.157 | 1.00 | 20.00 |
| ATOM | 1781 | CG1 | VAL | 500 | 27.349 | 4.028 | 74.498 | 1.00 | 20.00 |
| ATOM | 1782 | CG2 | VAL | 500 | 27.267 | 2.235 | 72.648 | 1.00 | 20.00 |
| ATOM | 1783 | C | VAL | 500 | 28.452 | 2.106 | 76.226 | 1.00 | 20.00 |
| ATOM | 1784 | O | VAL | 500 | 29.131 | 3.004 | 76.723 | 1.00 | 20.00 |
| ATOM | 1785 | N | SER | 501 | 27.643 | 1.306 | 76.956 | 1.00 | 20.00 |
| ATOM | 1787 | CA | SER | 501 | 27.519 | 1.440 | 78.381 | 1.00 | 20.00 |
| ATOM | 1788 | CB | SER | 501 | 26.337 | 2.321 | 78.819 | 1.00 | 20.00 |
| ATOM | 1789 | OG | SER | 501 | 26.279 | 2.402 | 80.235 | 1.00 | 20.00 |
| ATOM | 1791 | C | SER | 501 | 27.309 | 0.062 | 78.932 | 1.00 | 20.00 |
| ATOM | 1792 | O | SER | 501 | 27.178 | -0.900 | 78.175 | 1.00 | 20.00 |
| ATOM | 1793 | N | CYS | 502 | 27.269 | -0.068 | 80.277 | 1.00 | 20.00 |
| ATOM | 1795 | CA | CYS | 502 | 27.190 | -1.365 | 80.887 | 1.00 | 20.00 |
| ATOM | 1796 | CB | CYS | 502 | 28.384 | -1.609 | 81.830 | 1.00 | 20.00 |
| ATOM | 1797 | SG | CYS | 502 | 28.554 | -3.311 | 82.433 | 1.00 | 20.00 |
| ATOM | 1798 | C | CYS | 502 | 25.908 | -1.495 | 81.653 | 1.00 | 20.00 |
| ATOM | 1799 | O | CYS | 502 | 25.412 | -0.529 | 82.231 | 1.00 | 20.00 |
| ATOM | 1800 | N | ARG | 503 | 25.307 | -2.704 | 81.621 | 1.00 | 20.00 |
| ATOM | 1802 | CA | ARG | 503 | 24.084 | -2.958 | 82.327 | 1.00 | 20.00 |
| ATOM | 1803 | CB | ARG | 503 | 23.441 | -4.308 | 81.965 | 1.00 | 20.00 |
| ATOM | 1804 | CG | ARG | 503 | 22.036 | -4.476 | 82.549 | 1.00 | 20.00 |
| ATOM | 1805 | CD | ARG | 503 | 21.326 | -5.747 | 82.079 | 1.00 | 20.00 |
| ATOM | 1806 | NE | ARG | 503 | 21.250 | -5.684 | 80.591 | 1.00 | 20.00 |
| ATOM | 1808 | CZ | ARG | 503 | 20.221 | -5.027 | 79.980 | 1.00 | 20.00 |
| ATOM | 1809 | NH1 | ARG | 503 | 19.253 | -4.425 | 80.731 | 1.00 | 20.00 |
| ATOM | 1812 | NH2 | ARG | 503 | 20.160 | -4.971 | 78.618 | 1.00 | 20.00 |
| ATOM | 1815 | C | ARG | 503 | 24.343 | -2.949 | 83.798 | 1.00 | 20.00 |
| ATOM | 1816 | O | ARG | 503 | 23.570 | -2.388 | 84.573 | 1.00 | 20.00 |
| ATOM | 1817 | N | ASN | 504 | 25.466 | -3.564 | 84.211 | 1.00 | 20.00 |
| ATOM | 1819 | CA | ASN | 504 | 25.811 | -3.647 | 85.600 | 1.00 | 20.00 |
| ATOM | 1820 | CB | ASN | 504 | 26.210 | -5.061 | 86.059 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1821 | CG | ASN | 504 | 24.945 | -5.909 | 86.120 | 1.00 | 20.00 |
| ATOM | 1822 | OD1 | ASN | 504 | 24.548 | -6.522 | 85.131 | 1.00 | 20.00 |
| ATOM | 1823 | ND2 | ASN | 504 | 24.293 | -5.950 | 87.313 | 1.00 | 20.00 |
| ATOM | 1826 | C | ASN | 504 | 26.980 | -2.740 | 85.824 | 1.00 | 20.00 |
| ATOM | 1827 | O | ASN | 504 | 26.865 | -1.522 | 85.689 | 1.00 | 20.00 |
| ATOM | 1828 | N | VAL | 505 | 28.139 | -3.314 | 86.200 | 1.00 | 20.00 |
| ATOM | 1830 | CA | VAL | 505 | 29.288 | -2.505 | 86.489 | 1.00 | 20.00 |
| ATOM | 1831 | CB | VAL | 505 | 29.963 | -2.869 | 87.780 | 1.00 | 20.00 |
| ATOM | 1832 | CG1 | VAL | 505 | 28.979 | -2.620 | 88.935 | 1.00 | 20.00 |
| ATOM | 1833 | CG2 | VAL | 505 | 30.445 | -4.325 | 87.684 | 1.00 | 20.00 |
| ATOM | 1834 | C | VAL | 505 | 30.314 | -2.635 | 85.410 | 1.00 | 20.00 |
| ATOM | 1835 | O | VAL | 505 | 30.472 | -3.695 | 84.808 | 1.00 | 20.00 |
| ATOM | 1836 | N | SER | 506 | 31.038 | -1.534 | 85.132 | 1.00 | 20.00 |
| ATOM | 1838 | CA | SER | 506 | 32.047 | -1.574 | 84.117 | 1.00 | 20.00 |
| ATOM | 1839 | CB | SER | 506 | 32.071 | -0.323 | 83.220 | 1.00 | 20.00 |
| ATOM | 1840 | OG | SER | 506 | 33.101 | -0.437 | 82.250 | 1.00 | 20.00 |
| ATOM | 1842 | C | SER | 506 | 33.370 | -1.667 | 84.795 | 1.00 | 20.00 |
| ATOM | 1843 | O | SER | 506 | 33.630 | -0.956 | 85.765 | 1.00 | 20.00 |
| ATOM | 1844 | N | ARG | 507 | 34.236 | -2.583 | 84.319 | 1.00 | 20.00 |
| ATOM | 1846 | CA | ARG | 507 | 35.518 | -2.700 | 84.940 | 1.00 | 20.00 |
| ATOM | 1847 | CB | ARG | 507 | 35.551 | -3.770 | 86.044 | 1.00 | 20.00 |
| ATOM | 1848 | CG | ARG | 507 | 36.846 | -3.786 | 86.857 | 1.00 | 20.00 |
| ATOM | 1849 | CD | ARG | 507 | 38.033 | -4.429 | 86.137 | 1.00 | 20.00 |
| ATOM | 1850 | NE | ARG | 507 | 39.153 | -4.497 | 87.119 | 1.00 | 20.00 |
| ATOM | 1852 | CZ | ARG | 507 | 40.019 | -3.451 | 87.258 | 1.00 | 20.00 |
| ATOM | 1853 | NH1 | ARG | 507 | 41.011 | -3.511 | 88.194 | 1.00 | 20.00 |
| ATOM | 1856 | NH2 | ARG | 507 | 39.896 | -2.347 | 86.465 | 1.00 | 20.00 |
| ATOM | 1859 | C | ARG | 507 | 36.547 | -3.076 | 83.922 | 1.00 | 20.00 |
| ATOM | 1860 | O | ARG | 507 | 36.361 | -4.008 | 83.140 | 1.00 | 20.00 |
| ATOM | 1861 | N | GLY | 508 | 37.671 | -2.337 | 83.903 | 1.00 | 20.00 |
| ATOM | 1863 | CA | GLY | 508 | 38.761 | -2.667 | 83.032 | 1.00 | 20.00 |
| ATOM | 1864 | C | GLY | 508 | 38.308 | -2.741 | 81.610 | 1.00 | 20.00 |
| ATOM | 1865 | O | GLY | 508 | 38.630 | -3.693 | 80.902 | 1.00 | 20.00 |
| ATOM | 1866 | N | ARG | 509 | 37.533 | -1.743 | 81.151 | 1.00 | 20.00 |
| ATOM | 1868 | CA | ARG | 509 | 37.133 | -1.717 | 79.773 | 1.00 | 20.00 |
| ATOM | 1869 | CB | ARG | 509 | 38.342 | -1.804 | 78.826 | 1.00 | 20.00 |
| ATOM | 1870 | CG | ARG | 509 | 39.300 | -0.620 | 78.975 | 1.00 | 20.00 |
| ATOM | 1871 | CD | ARG | 509 | 40.611 | -0.784 | 78.205 | 1.00 | 20.00 |
| ATOM | 1872 | NE | ARG | 509 | 40.319 | -0.592 | 76.758 | 1.00 | 20.00 |
| ATOM | 1874 | CZ | ARG | 509 | 41.257 | -0.011 | 75.954 | 1.00 | 20.00 |
| ATOM | 1875 | NH1 | ARG | 509 | 41.009 | 0.154 | 74.622 | 1.00 | 20.00 |
| ATOM | 1878 | NH2 | ARG | 509 | 42.441 | 0.412 | 76.486 | 1.00 | 20.00 |
| ATOM | 1881 | C | ARG | 509 | 36.214 | -2.859 | 79.461 | 1.00 | 20.00 |
| ATOM | 1882 | O | ARG | 509 | 35.901 | -3.104 | 78.297 | 1.00 | 20.00 |
| ATOM | 1883 | N | GLU | 510 | 35.726 | -3.579 | 80.491 | 1.00 | 20.00 |
| ATOM | 1885 | CA | GLU | 510 | 34.853 | -4.686 | 80.217 | 1.00 | 20.00 |
| ATOM | 1886 | CB | GLU | 510 | 35.456 | -6.027 | 80.669 | 1.00 | 20.00 |
| ATOM | 1887 | CG | GLU | 510 | 36.723 | -6.393 | 79.890 | 1.00 | 20.00 |
| ATOM | 1888 | CD | GLU | 510 | 37.447 | -7.508 | 80.630 | 1.00 | 20.00 |
| ATOM | 1889 | OE1 | GLU | 510 | 37.664 | -8.583 | 80.009 | 1.00 | 20.00 |
| ATOM | 1890 | OE2 | GLU | 510 | 37.801 | -7.298 | 81.821 | 1.00 | 20.00 |
| ATOM | 1891 | C | GLU | 510 | 33.589 | -4.481 | 80.984 | 1.00 | 20.00 |
| ATOM | 1892 | O | GLU | 510 | 33.600 | -3.976 | 82.105 | 1.00 | 20.00 |
| ATOM | 1893 | N | CYS | 511 | 32.451 | -4.875 | 80.385 | 1.00 | 20.00 |
| ATOM | 1895 | CA | CYS | 511 | 31.191 | -4.703 | 81.042 | 1.00 | 20.00 |
| ATOM | 1896 | CB | CYS | 511 | 30.037 | -4.512 | 80.039 | 1.00 | 20.00 |
| ATOM | 1897 | SG | CYS | 511 | 28.372 | -4.452 | 80.762 | 1.00 | 20.00 |
| ATOM | 1898 | C | CYS | 511 | 30.961 | -5.930 | 81.858 | 1.00 | 20.00 |
| ATOM | 1899 | O | CYS | 511 | 30.691 | -7.003 | 81.320 | 1.00 | 20.00 |
| ATOM | 1900 | N | VAL | 512 | 31.079 | -5.786 | 83.195 | 1.00 | 20.00 |
| ATOM | 1902 | CA | VAL | 512 | 30.909 | -6.884 | 84.104 | 1.00 | 20.00 |
| ATOM | 1903 | CB | VAL | 512 | 31.969 | -6.991 | 85.164 | 1.00 | 20.00 |
| ATOM | 1904 | CG1 | VAL | 512 | 33.231 | -7.611 | 84.562 | 1.00 | 20.00 |
| ATOM | 1905 | CG2 | VAL | 512 | 32.239 | -5.583 | 85.710 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|
| ATOM | 1906 | C | VAL | 512 | 29.591 | -6.838 | 84.803 | 1.00 | 20.00 |
| ATOM | 1907 | O | VAL | 512 | 29.045 | -5.775 | 85.096 | 1.00 | 20.00 |
| ATOM | 1908 | N | ASP | 513 | 29.025 | -8.039 | 85.028 | 1.00 | 20.00 |
| i 4 | 1910 | CA | ASP | 513 | 27.799 | -8.215 | 85.747 | 1.00 | 20.00 |
| ATOM | 1911 | CB | ASP | 513 | 27.233 | -9.641 | 85.627 | 1.00 | 20.00 |
| ATOM | 1912 | CG | ASP | 513 | 28.270 | -10.614 | 86.169 | 1.00 | 20.00 |
| ATOM | 1913 | OD1 | ASP | 513 | 28.030 | -11.193 | 87.262 | 1.00 | 20.00 |
| ATOM | 1914 | OD2 | ASP | 513 | 29.313 | -10.800 | 85.487 | 1.00 | 20.00 |
| ATOM | 1915 | C | ASP | 513 | 28.029 | -7.927 | 87.193 | 1.00 | 20.00 |
| ATOM | 1916 | O | ASP | 513 | 27.143 | -7.429 | 87.887 | 1.00 | 20.00 |
| ATOM | 1917 | N | LYS | 514 | 29.224 | -8.282 | 87.700 | 1.00 | 20.00 |
| ATOM | 1919 | CA | LYS | 514 | 29.519 | -8.023 | 89.077 | 1.00 | 20.00 |
| ATOM | 1920 | CB | LYS | 514 | 29.130 | -9.178 | 90.019 | 1.00 | 20.00 |
| ATOM | 1921 | CG | LYS | 514 | 29.727 | -10.535 | 89.641 | 1.00 | 20.00 |
| ATOM | 1922 | CD | LYS | 514 | 31.238 | -10.640 | 89.842 | 1.00 | 20.00 |
| ATOM | 1923 | CE | LYS | 514 | 31.789 | -12.028 | 89.510 | 1.00 | 20.00 |
| ATOM | 1924 | NZ | LYS | 514 | 31.203 | -13.034 | 90.424 | 1.00 | 20.00 |
| ATOM | 1928 | C | LYS | 514 | 30.987 | -7.772 | 89.197 | 1.00 | 20.00 |
| ATOM | 1929 | O | LYS | 514 | 31.771 | -8.128 | 88.318 | 1.00 | 20.00 |
| ATOM | 1930 | N | CYS | 515 | 31.388 | -7.130 | 90.309 | 1.00 | 20.00 |
| ATOM | 1932 | CA | CYS | 515 | 32.760 | -6.793 | 90.544 | 1.00 | 20.00 |
| ATOM | 1933 | CB | CYS | 515 | 32.987 | -6.056 | 91.874 | 1.00 | 20.00 |
| ATOM | 1934 | SG | CYS | 515 | 32.657 | -4.275 | 91.855 | 1.00 | 20.00 |
| ATOM | 1935 | C | CYS | 515 | 33.608 | -8.019 | 90.651 | 1.00 | 20.00 |
| ATOM | 1936 | O | CYS | 515 | 33.193 | -9.045 | 91.187 | 1.00 | 20.00 |
| ATOM | 1937 | N | LYS | 516 | 34.854 | -7.916 | 90.148 | 1.00 | 20.00 |
| ATOM | 1939 | CA | LYS | 516 | 35.779 | -9.006 | 90.231 | 1.00 | 20.00 |
| ATOM | 1940 | CB | LYS | 516 | 36.980 | -8.859 | 89.281 | 1.00 | 20.00 |
| ATOM | 1941 | CG | LYS | 516 | 36.574 | -8.714 | 87.813 | 1.00 | 20.00 |
| ATOM | 1942 | CD | LYS | 516 | 35.721 | -9.868 | 87.279 | 1.00 | 20.00 |
| ATOM | 1943 | CE | LYS | 516 | 36.519 | -11.130 | 86.944 | 1.00 | 20.00 |
| ATOM | 1944 | NZ | LYS | 516 | 35.616 | -12.169 | 86.398 | 1.00 | 20.00 |
| ATOM | 1948 | C | LYS | 516 | 36.308 | -8.986 | 91.632 | 1.00 | 20.00 |
| ATOM | 1949 | O | LYS | 516 | 36.045 | -8.054 | 92.389 | 1.00 | 20.00 |
| ATOM | 1950 | N | LEU | 517 | 37.070 | -10.024 | 92.024 | 1.00 | 20.00 |
| ATOM | 1952 | CA | LEU | 517 | 37.576 | -10.086 | 93.364 | 1.00 | 20.00 |
| ATOM | 1953 | CB | LEU | 517 | 38.331 | -11.391 | 93.662 | 1.00 | 20.00 |
| ATOM | 1954 | CG | LEU | 517 | 37.452 | -12.646 | 93.499 | 1.00 | 20.00 |
| ATOM | 1955 | CD1 | LEU | 517 | 38.242 | -13.929 | 93.807 | 1.00 | 20.00 |
| ATOM | 1956 | CD2 | LEU | 517 | 36.158 | -12.536 | 94.320 | 1.00 | 20.00 |
| ATOM | 1957 | C | LEU | 517 | 38.532 | -8.949 | 93.545 | 1.00 | 20.00 |
| ATOM | 1958 | O | LEU | 517 | 39.091 | -8.440 | 92.575 | 1.00 | 20.00 |
| ATOM | 1959 | N | LEU | 518 | 38.719 | -8.513 | 94.809 | 1.00 | 20.00 |
| ATOM | 1961 | CA | LEU | 518 | 39.625 | -7.448 | 95.142 | 1.00 | 20.00 |
| ATOM | 1962 | CB | LEU | 518 | 40.947 | -7.494 | 94.355 | 1.00 | 20.00 |
| ATOM | 1963 | CG | LEU | 518 | 41.918 | -6.351 | 94.714 | 1.00 | 20.00 |
| ATOM | 1964 | CD1 | LEU | 518 | 42.433 | -6.480 | 96.156 | 1.00 | 20.00 |
| ATOM | 1965 | CD2 | LEU | 518 | 43.044 | -6.226 | 93.676 | 1.00 | 20.00 |
| ATOM | 1966 | C | LEU | 518 | 38.997 | -6.114 | 94.879 | 1.00 | 20.00 |
| ATOM | 1967 | O | LEU | 518 | 39.208 | -5.171 | 95.640 | 1.00 | 20.00 |
| ATOM | 1968 | N | GLU | 519 | 38.191 | -5.992 | 93.804 | 1.00 | 20.00 |
| ATOM | 1970 | CA | GLU | 519 | 37.604 | -4.713 | 93.517 | 1.00 | 20.00 |
| ATOM | 1971 | CB | GLU | 519 | 37.515 | -4.360 | 92.020 | 1.00 | 20.00 |
| ATOM | 1972 | CG | GLU | 519 | 38.842 | -3.943 | 91.381 | 1.00 | 20.00 |
| ATOM | 1973 | CD | GLU | 519 | 39.585 | -5.191 | 90.933 | 1.00 | 20.00 |
| ATOM | 1974 | OE1 | GLU | 519 | 38.935 | -6.078 | 90.320 | 1.00 | 20.00 |
| ATOM | 1975 | OE2 | GLU | 519 | 40.814 | -5.272 | 91.196 | 1.00 | 20.00 |
| ATOM | 1976 | C | GLU | 519 | 36.208 | -4.674 | 94.044 | 1.00 | 20.00 |
| ATOM | 1977 | O | GLU | 519 | 35.528 | -5.696 | 94.136 | 1.00 | 20.00 |
| ATOM | 1978 | N | GLY | 520 | 35.758 | -3.463 | 94.422 | 1.00 | 20.00 |
| ATOM | 1980 | CA | GLY | 520 | 34.439 | -3.272 | 94.938 | 1.00 | 20.00 |
| ATOM | 1981 | C | GLY | 520 | 33.813 | -2.189 | 94.136 | 1.00 | 20.00 |
| ATOM | 1982 | O | GLY | 520 | 34.491 | -1.278 | 93.667 | 1.00 | 20.00 |
| ATOM | 1983 | N | GLU | 521 | 32.483 | -2.262 | 93.968 | 1.00 | 40.00 |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|
| ATOM | 1985 | CA | GLU | 521 | 31.802 | -1.288 | 93.176 | 1.00 | 40.00 |
| ATOM | 1986 | CB | GLU | 521 | 30.416 | -1.771 | 92.716 | 1.00 | 40.00 |
| ATOM | 1987 | CG | GLU | 521 | 29.514 | -2.180 | 93.882 | 1.00 | 40.00 |
| ATOM | 1988 | CD | GLU | 521 | 28.220 | -2.746 | 93.314 | 1.00 | 40.00 |
| ATOM | 1989 | OE1 | GLU | 521 | 27.535 | -3.502 | 94.053 | 1.00 | 40.00 |
| ATOM | 1990 | OE2 | GLU | 521 | 27.901 | -2.435 | 92.135 | 1.00 | 40.00 |
| ATOM | 1991 | C | GLU | 521 | 31.612 | -0.046 | 93.973 | 1.00 | 40.00 |
| ATOM | 1992 | O | GLU | 521 | 31.258 | -0.082 | 95.150 | 1.00 | 40.00 |
| ATOM | 1993 | N | PRO | 522 | 31.876 | 1.066 | 93.349 | 1.00 | 40.00 |
| ATOM | 1994 | CD | PRO | 522 | 33.036 | 1.177 | 92.484 | 1.00 | 40.00 |
| ATOM | 1995 | CA | PRO | 522 | 31.617 | 2.298 | 94.026 | 1.00 | 40.00 |
| ATOM | 1996 | CB | PRO | 522 | 32.447 | 3.373 | 93.318 | 1.00 | 40.00 |
| ATOM | 1997 | CG | PRO | 522 | 33.044 | 2.661 | 92.089 | 1.00 | 40.00 |
| ATOM | 1998 | C | PRO | 522 | 30.143 | 2.511 | 94.004 | 1.00 | 40.00 |
| ATOM | 1999 | O | PRO | 522 | 29.528 | 2.289 | 92.962 | 1.00 | 40.00 |
| ATOM | 2000 | N | ARG | 523 | 29.558 | 2.927 | 95.142 | 1.00 | 60.00 |
| ATOM | 2002 | CA | ARG | 523 | 28.138 | 3.104 | 95.212 | 1.00 | 60.00 |
| ATOM | 2003 | CB | ARG | 523 | 27.632 | 3.334 | 96.647 | 1.00 | 60.00 |
| ATOM | 2004 | CG | ARG | 523 | 27.668 | 2.065 | 97.500 | 1.00 | 60.00 |
| ATOM | 2005 | CD | ARG | 523 | 26.622 | 1.037 | 97.064 | 1.00 | 60.00 |
| ATOM | 2006 | NE | ARG | 523 | 26.744 | -0.152 | 97.951 | 1.00 | 60.00 |
| ATOM | 2008 | CZ | ARG | 523 | 25.823 | -1.155 | 97.856 | 1.00 | 60.00 |
| ATOM | 2009 | NH1 | ARG | 523 | 24.792 | -1.047 | 96.968 | 1.00 | 60.00 |
| ATOM | 2012 | NH2 | ARG | 523 | 25.934 | -2.264 | 98.645 | 1.00 | 60.00 |
| ATOM | 2015 | C | ARG | 523 | 27.691 | 4.256 | 94.375 | 1.00 | 60.00 |
| ATOM | 2016 | O | ARG | 523 | 26.770 | 4.121 | 93.570 | 1.00 | 60.00 |
| ATOM | 2017 | N | GLU | 524 | 28.341 | 5.425 | 94.525 | 1.00 | 60.00 |
| ATOM | 2019 | CA | GLU | 524 | 27.889 | 6.552 | 93.767 | 1.00 | 60.00 |
| ATOM | 2020 | CB | GLU | 524 | 28.307 | 7.917 | 94.338 | 1.00 | 60.00 |
| ATOM | 2021 | CG | GLU | 524 | 29.821 | 8.130 | 94.358 | 1.00 | 60.00 |
| ATOM | 2022 | CD | GLU | 524 | 30.077 | 9.592 | 94.694 | 1.00 | 60.00 |
| ATOM | 2023 | OE1 | GLU | 524 | 29.169 | 10.425 | 94.430 | 1.00 | 60.00 |
| ATOM | 2024 | OE2 | GLU | 524 | 31.183 | 9.896 | 95.214 | 1.00 | 60.00 |
| ATOM | 2025 | C | GLU | 524 | 28.463 | 6.463 | 92.398 | 1.00 | 60.00 |
| ATOM | 2026 | O | GLU | 524 | 29.462 | 5.782 | 92.170 | 1.00 | 60.00 |
| ATOM | 2027 | N | PHE | 525 | 27.807 | 7.140 | 91.438 | 1.00 | 60.00 |
| ATOM | 2029 | CA | PHE | 525 | 28.296 | 7.136 | 90.096 | 1.00 | 60.00 |
| ATOM | 2030 | CB | PHE | 525 | 27.511 | 6.173 | 89.180 | 1.00 | 60.00 |
| ATOM | 2031 | CG | PHE | 525 | 26.062 | 6.520 | 89.262 | 1.00 | 60.00 |
| ATOM | 2032 | CD1 | PHE | 525 | 25.327 | 6.139 | 90.361 | 1.00 | 60.00 |
| ATOM | 2033 | CD2 | PHE | 525 | 25.421 | 7.158 | 88.224 | 1.00 | 60.00 |
| ATOM | 2034 | CE1 | PHE | 525 | 23.986 | 6.428 | 90.447 | 1.00 | 60.00 |
| ATOM | 2035 | CE2 | PHE | 525 | 24.079 | 7.449 | 88.302 | 1.00 | 60.00 |
| ATOM | 2036 | CZ | PHE | 525 | 23.361 | 7.094 | 89.419 | 1.00 | 60.00 |
| ATOM | 2037 | C | PHE | 525 | 28.221 | 8.522 | 89.541 | 1.00 | 60.00 |
| ATOM | 2038 | O | PHE | 525 | 27.144 | 9.036 | 89.244 | 1.00 | 60.00 |
| ATOM | 2039 | N | VAL | 526 | 29.385 | 9.185 | 89.416 | 1.00 | 60.00 |
| ATOM | 2041 | CA | VAL | 526 | 29.371 | 10.481 | 88.812 | 1.00 | 60.00 |
| ATOM | 2042 | CB | VAL | 526 | 30.667 | 11.230 | 88.964 | 1.00 | 60.00 |
| ATOM | 2043 | CG1 | VAL | 526 | 31.810 | 10.425 | 88.324 | 1.00 | 60.00 |
| ATOM | 2044 | CG2 | VAL | 526 | 30.481 | 12.633 | 88.360 | 1.00 | 60.00 |
| ATOM | 2045 | C | VAL | 526 | 29.111 | 10.214 | 87.369 | 1.00 | 60.00 |
| ATOM | 2046 | O | VAL | 526 | 28.324 | 10.904 | 86.722 | 1.00 | 60.00 |
| ATOM | 2047 | N | GLU | 527 | 29.766 | 9.165 | 86.840 | 1.00 | 60.00 |
| ATOM | 2049 | CA | GLU | 527 | 29.567 | 8.755 | 85.486 | 1.00 | 60.00 |
| ATOM | 2050 | CB | GLU | 527 | 30.877 | 8.509 | 84.718 | 1.00 | 60.00 |
| ATOM | 2051 | CG | GLU | 527 | 31.745 | 7.401 | 85.318 | 1.00 | 60.00 |
| ATOM | 2052 | CD | GLU | 527 | 32.996 | 7.277 | 84.460 | 1.00 | 60.00 |
| ATOM | 2053 | OE1 | GLU | 527 | 33.118 | 8.051 | 83.473 | 1.00 | 60.00 |
| ATOM | 2054 | OE2 | GLU | 527 | 33.850 | 6.407 | 84.782 | 1.00 | 60.00 |
| ATOM | 2055 | C | GLU | 527 | 28.852 | 7.454 | 85.613 | 1.00 | 60.00 |
| ATOM | 2056 | O | GLU | 527 | 28.059 | 7.264 | 86.534 | 1.00 | 60.00 |
| ATOM | 2057 | N | ASN | 528 | 29.098 | 6.517 | 84.682 | 1.00 | 60.00 |
| ATOM | 2059 | CA | ASN | 528 | 28.438 | 5.254 | 84.795 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2060 | CB | ASN | 528 | 28.583 | 4.372 | 83.545 | 1.00 | 60.00 |
| ATOM | 2061 | CG | ASN | 528 | 27.745 | 5.007 | 82.446 | 1.00 | 60.00 |
| ATOM | 2062 | OD1 | ASN | 528 | 28.080 | 6.064 | 81.915 | 1.00 | 60.00 |
| ATOM | 2063 | ND2 | ASN | 528 | 26.613 | 4.339 | 82.093 | 1.00 | 60.00 |
| ATOM | 2066 | C | ASN | 528 | 29.058 | 4.542 | 85.951 | 1.00 | 60.00 |
| ATOM | 2067 | O | ASN | 528 | 30.106 | 4.946 | 86.451 | 1.00 | 60.00 |
| ATOM | 2068 | N | SER | 529 | 28.404 | 3.462 | 86.420 | 1.00 | 60.00 |
| ATOM | 2070 | CA | SER | 529 | 28.932 | 2.745 | 87.541 | 1.00 | 60.00 |
| ATOM | 2071 | CB | SER | 529 | 27.912 | 1.823 | 88.230 | 1.00 | 60.00 |
| ATOM | 2072 | OG | SER | 529 | 26.889 | 2.597 | 88.837 | 1.00 | 60.00 |
| ATOM | 2074 | C | SER | 529 | 30.065 | 1.899 | 87.074 | 1.00 | 60.00 |
| ATOM | 2075 | O | SER | 529 | 30.100 | 1.453 | 85.928 | 1.00 | 60.00 |
| ATOM | 2076 | N | GLU | 530 | 31.040 | 1.679 | 87.972 | 1.00 | 40.00 |
| ATOM | 2078 | CA | GLU | 530 | 32.187 | 0.891 | 87.648 | 1.00 | 40.00 |
| ATOM | 2079 | CB | GLU | 530 | 33.402 | 1.722 | 87.198 | 1.00 | 40.00 |
| ATOM | 2080 | CG | GLU | 530 | 33.230 | 2.428 | 85.852 | 1.00 | 40.00 |
| ATOM | 2081 | CD | GLU | 530 | 34.477 | 3.269 | 85.618 | 1.00 | 40.00 |
| ATOM | 2082 | OE1 | GLU | 530 | 34.663 | 3.755 | 84.470 | 1.00 | 40.00 |
| ATOM | 2083 | OE2 | GLU | 530 | 35.262 | 3.437 | 86.590 | 1.00 | 40.00 |
| ATOM | 2084 | C | GLU | 530 | 32.595 | 0.225 | 88.914 | 1.00 | 40.00 |
| ATOM | 2085 | O | GLU | 530 | 31.996 | 0.441 | 89.966 | 1.00 | 40.00 |
| ATOM | 2086 | N | CYS | 531 | 33.630 | -0.629 | 88.833 | 1.00 | 20.00 |
| ATOM | 2088 | CA | CYS | 531 | 34.103 | -1.267 | 90.016 | 1.00 | 20.00 |
| ATOM | 2089 | CB | CYS | 531 | 34.350 | -2.774 | 89.869 | 1.00 | 20.00 |
| ATOM | 2090 | SG | CYS | 531 | 34.511 | -3.530 | 91.504 | 1.00 | 20.00 |
| ATOM | 2091 | C | CYS | 531 | 35.424 | -0.624 | 90.264 | 1.00 | 20.00 |
| ATOM | 2092 | O | CYS | 531 | 36.142 | -0.277 | 89.328 | 1.00 | 20.00 |
| ATOM | 2093 | N | ILE | 532 | 35.769 | -0.436 | 91.548 | 1.00 | 20.00 |
| ATOM | 2095 | CA | ILE | 532 | 36.989 | 0.225 | 91.890 | 1.00 | 20.00 |
| ATOM | 2096 | CB | ILE | 532 | 36.762 | 1.494 | 92.659 | 1.00 | 20.00 |
| ATOM | 2097 | CG2 | ILE | 532 | 36.068 | 1.136 | 93.983 | 1.00 | 20.00 |
| ATOM | 2098 | CG1 | ILE | 532 | 38.073 | 2.277 | 92.821 | 1.00 | 20.00 |
| ATOM | 2099 | CD1 | ILE | 532 | 37.862 | 3.702 | 93.330 | 1.00 | 20.00 |
| ATOM | 2100 | C | ILE | 532 | 37.797 | -0.698 | 92.746 | 1.00 | 20.00 |
| ATOM | 2101 | O | ILE | 532 | 37.286 | -1.694 | 93.251 | 1.00 | 20.00 |
| ATOM | 2102 | N | GLN | 533 | 39.099 | -0.398 | 92.911 | 1.00 | 20.00 |
| ATOM | 2104 | CA | GLN | 533 | 39.970 | -1.243 | 93.677 | 1.00 | 20.00 |
| ATOM | 2105 | CB | GLN | 533 | 41.456 | -1.010 | 93.368 | 1.00 | 20.00 |
| ATOM | 2106 | CG | GLN | 533 | 41.913 | 0.404 | 93.730 | 1.00 | 20.00 |
| ATOM | 2107 | CD | GLN | 533 | 43.389 | 0.531 | 93.386 | 1.00 | 20.00 |
| ATOM | 2108 | OE1 | GLN | 533 | 44.031 | -0.438 | 92.983 | 1.00 | 20.00 |
| ATOM | 2109 | NE2 | GLN | 533 | 43.948 | 1.759 | 93.553 | 1.00 | 20.00 |
| ATOM | 2112 | C | GLN | 533 | 39.798 | -0.994 | 95.138 | 1.00 | 20.00 |
| ATOM | 2113 | O | GLN | 533 | 39.414 | 0.096 | 95.558 | 1.00 | 20.00 |
| ATOM | 2114 | N | CYS | 534 | 40.071 | -2.031 | 95.955 | 1.00 | 20.00 |
| ATOM | 2116 | CA | CYS | 534 | 40.010 | -1.852 | 97.371 | 1.00 | 20.00 |
| ATOM | 2117 | CB | CYS | 534 | 39.102 | -2.844 | 98.131 | 1.00 | 20.00 |
| ATOM | 2118 | SG | CYS | 534 | 37.326 | -2.688 | 97.744 | 1.00 | 20.00 |
| ATOM | 2119 | C | CYS | 534 | 41.410 | -2.018 | 97.894 | 1.00 | 20.00 |
| ATOM | 2120 | O | CYS | 534 | 42.283 | -2.538 | 97.200 | 1.00 | 20.00 |
| ATOM | 2121 | N | HIS | 535 | 41.663 | -1.554 | 99.138 | 1.00 | 20.00 |
| ATOM | 2123 | CA | HIS | 535 | 42.975 | -1.624 | 99.726 | 1.00 | 20.00 |
| ATOM | 2124 | CB | HIS | 535 | 43.142 | -0.690 | 100.943 | 1.00 | 20.00 |
| ATOM | 2125 | CG | HIS | 535 | 44.548 | -0.614 | 101.466 | 1.00 | 20.00 |
| ATOM | 2126 | CD2 | HIS | 535 | 45.604 | 0.126 | 101.031 | 1.00 | 20.00 |
| ATOM | 2127 | ND1 | HIS | 535 | 45.030 | -1.377 | 102.507 | 1.00 | 20.00 |
| ATOM | 2129 | CE1 | HIS | 535 | 46.342 | -1.063 | 102.649 | 1.00 | 20.00 |
| ATOM | 2130 | NE2 | HIS | 535 | 46.737 | -0.155 | 101.775 | 1.00 | 20.00 |
| ATOM | 2132 | C | HIS | 535 | 43.233 | -3.033 | 100.155 | 1.00 | 20.00 |
| ATOM | 2133 | O | HIS | 535 | 42.305 | -3.815 | 100.356 | 1.00 | 20.00 |
| ATOM | 2134 | N | PRO | 536 | 44.486 | -3.387 | 100.264 | 1.00 | 20.00 |
| ATOM | 2135 | CD | PRO | 536 | 45.537 | -2.747 | 99.494 | 1.00 | 20.00 |
| ATOM | 2136 | CA | PRO | 536 | 44.852 | -4.717 | 100.662 | 1.00 | 20.00 |
| ATOM | 2137 | CB | PRO | 536 | 46.357 | -4.843 | 100.391 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2138 | CG | PRO | 536 | 46.816 | -3.419 | 100.015 | 1.00 | 20.00 |
| ATOM | 2139 | C | PRO | 536 | 44.427 | -5.022 | 102.064 | 1.00 | 20.00 |
| ATOM | 2140 | O | PRO | 536 | 44.167 | -6.187 | 102.364 | 1.00 | 20.00 |
| ATOM | 2141 | N | GLU | 537 | 44.390 | -4.005 | 102.944 | 1.00 | 20.00 |
| ATOM | 2143 | CA | GLU | 537 | 43.977 | -4.177 | 104.307 | 1.00 | 20.00 |
| ATOM | 2144 | CB | GLU | 537 | 44.378 | -2.999 | 105.211 | 1.00 | 20.00 |
| ATOM | 2145 | CG | GLU | 537 | 45.885 | -2.933 | 105.478 | 1.00 | 20.00 |
| ATOM | 2146 | CD | GLU | 537 | 46.253 | -4.093 | 106.397 | 1.00 | 20.00 |
| ATOM | 2147 | OE1 | GLU | 537 | 45.370 | -4.525 | 107.186 | 1.00 | 20.00 |
| ATOM | 2148 | OE2 | GLU | 537 | 47.420 | -4.562 | 106.324 | 1.00 | 20.00 |
| ATOM | 2149 | C | GLU | 537 | 42.503 | -4.368 | 104.422 | 1.00 | 20.00 |
| ATOM | 2150 | O | GLU | 537 | 42.021 | -5.109 | 105.278 | 1.00 | 20.00 |
| ATOM | 2151 | N | CYS | 538 | 41.750 | -3.673 | 103.557 | 1.00 | 20.00 |
| ATOM | 2153 | CA | CYS | 538 | 40.321 | -3.717 | 103.554 | 1.00 | 20.00 |
| ATOM | 2154 | CB | CYS | 538 | 39.797 | -3.005 | 102.292 | 1.00 | 20.00 |
| ATOM | 2155 | SG | CYS | 538 | 37.999 | -2.970 | 102.127 | 1.00 | 20.00 |
| ATOM | 2156 | C | CYS | 538 | 39.911 | -5.156 | 103.539 | 1.00 | 20.00 |
| ATOM | 2157 | O | CYS | 538 | 40.518 | -5.975 | 102.854 | 1.00 | 20.00 |
| ATOM | 2158 | N | LEU | 539 | 38.889 | -5.507 | 104.347 | 1.00 | 60.00 |
| ATOM | 2160 | CA | LEU | 539 | 38.409 | -6.852 | 104.428 | 1.00 | 60.00 |
| ATOM | 2161 | CB | LEU | 539 | 38.406 | -7.409 | 105.860 | 1.00 | 60.00 |
| ATOM | 2162 | CG | LEU | 539 | 37.889 | -8.855 | 105.959 | 1.00 | 60.00 |
| ATOM | 2163 | CD1 | LEU | 539 | 38.825 | -9.831 | 105.231 | 1.00 | 60.00 |
| ATOM | 2164 | CD2 | LEU | 539 | 37.635 | -9.253 | 107.421 | 1.00 | 60.00 |
| ATOM | 2165 | C | LEU | 539 | 36.994 | -6.842 | 103.954 | 1.00 | 60.00 |
| ATOM | 2166 | O | LEU | 539 | 36.240 | -5.889 | 104.147 | 1.00 | 60.00 |
| ATOM | 2167 | N | PRO | 540 | 36.662 | -7.905 | 103.289 | 1.00 | 60.00 |
| ATOM | 2168 | CD | PRO | 540 | 37.663 | -8.584 | 102.484 | 1.00 | 60.00 |
| ATOM | 2169 | CA | PRO | 540 | 35.343 | -8.046 | 102.736 | 1.00 | 60.00 |
| ATOM | 2170 | CB | PRO | 540 | 35.489 | -8.938 | 101.512 | 1.00 | 60.00 |
| ATOM | 2171 | CG | PRO | 540 | 36.865 | -9.605 | 101.667 | 1.00 | 60.00 |
| ATOM | 2172 | C | PRO | 540 | 34.342 | -8.599 | 103.690 | 1.00 | 60.00 |
| ATOM | 2173 | O | PRO | 540 | 34.718 | -9.251 | 104.661 | 1.00 | 60.00 |
| ATOM | 2174 | N | GLN | 541 | 33.050 | -8.358 | 103.404 | 1.00 | 60.00 |
| ATOM | 2176 | CA | GLN | 541 | 31.990 | -8.912 | 104.186 | 1.00 | 60.00 |
| ATOM | 2177 | CB | GLN | 541 | 30.807 | -7.956 | 104.410 | 1.00 | 60.00 |
| ATOM | 2178 | CG | GLN | 541 | 31.077 | -6.867 | 105.446 | 1.00 | 60.00 |
| ATOM | 2179 | CD | GLN | 541 | 31.039 | -7.529 | 106.816 | 1.00 | 60.00 |
| ATOM | 2180 | OE1 | GLN | 541 | 31.871 | -8.379 | 107.132 | 1.00 | 60.00 |
| ATOM | 2181 | NE2 | GLN | 541 | 30.039 | -7.140 | 107.650 | 1.00 | 60.00 |
| ATOM | 2184 | C | GLN | 541 | 31.472 | -10.050 | 103.379 | 1.00 | 60.00 |
| ATOM | 2185 | O | GLN | 541 | 32.239 | -10.843 | 102.837 | 1.00 | 60.00 |
| ATOM | 2186 | N | ALA | 542 | 30.135 | -10.148 | 103.275 | 1.00 | 60.00 |
| ATOM | 2188 | CA | ALA | 542 | 29.543 | -11.216 | 102.532 | 1.00 | 60.00 |
| ATOM | 2189 | CB | ALA | 542 | 28.010 | -11.108 | 102.452 | 1.00 | 60.00 |
| ATOM | 2190 | C | ALA | 542 | 30.081 | -11.120 | 101.144 | 1.00 | 60.00 |
| ATOM | 2191 | O | ALA | 542 | 30.434 | -12.127 | 100.533 | 1.00 | 60.00 |
| ATOM | 2192 | N | MET | 543 | 30.177 | -9.886 | 100.617 | 1.00 | 60.00 |
| ATOM | 2194 | CA | MET | 543 | 30.686 | -9.713 | 99.290 | 1.00 | 60.00 |
| ATOM | 2195 | CB | MET | 543 | 30.785 | -8.239 | 98.861 | 1.00 | 60.00 |
| ATOM | 2196 | CG | MET | 543 | 31.247 | -8.054 | 97.416 | 1.00 | 60.00 |
| ATOM | 2197 | SD | MET | 543 | 30.011 | -8.524 | 96.170 | 1.00 | 60.00 |
| ATOM | 2198 | CE | MET | 543 | 28.880 | -7.154 | 96.548 | 1.00 | 60.00 |
| ATOM | 2199 | C | MET | 543 | 32.060 | -10.297 | 99.248 | 1.00 | 60.00 |
| ATOM | 2200 | O | MET | 543 | 32.648 | -10.610 | 100.282 | 1.00 | 60.00 |
| ATOM | 2201 | N | ASN | 544 | 32.598 | -10.480 | 98.026 | 1.00 | 60.00 |
| ATOM | 2203 | CA | ASN | 544 | 33.905 | -11.044 | 97.865 | 1.00 | 60.00 |
| ATOM | 2204 | CB | ASN | 544 | 34.265 | -11.292 | 96.389 | 1.00 | 60.00 |
| ATOM | 2205 | CG | ASN | 544 | 34.181 | -9.971 | 95.639 | 1.00 | 60.00 |
| ATOM | 2206 | OD1 | ASN | 544 | 35.191 | -9.411 | 95.218 | 1.00 | 60.00 |
| ATOM | 2207 | ND2 | ASN | 544 | 32.934 | -9.453 | 95.470 | 1.00 | 60.00 |
| ATOM | 2210 | C | ASN | 544 | 34.920 | -10.129 | 98.468 | 1.00 | 60.00 |
| ATOM | 2211 | O | ASN | 544 | 35.778 | -10.570 | 99.231 | 1.00 | 60.00 |
| ATOM | 2212 | N | ILE | 545 | 34.851 | -8.826 | 98.131 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2214 | CA | ILE | 545 | 35.738 | -7.858 | 98.706 | 1.00 | 60.00 |
| ATOM | 2215 | CB | ILE | 545 | 36.858 | -7.450 | 97.791 | 1.00 | 60.00 |
| ATOM | 2216 | CG2 | ILE | 545 | 36.259 | -6.690 | 96.596 | 1.00 | 60.00 |
| ATOM | 2217 | CG1 | ILE | 545 | 37.926 | -6.670 | 98.574 | 1.00 | 60.00 |
| ATOM | 2218 | CD1 | ILE | 545 | 38.669 | -7.527 | 99.599 | 1.00 | 60.00 |
| ATOM | 2219 | C | ILE | 545 | 34.872 | -6.670 | 98.974 | 1.00 | 60.00 |
| ATOM | 2220 | O | ILE | 545 | 34.027 | -6.327 | 98.149 | 1.00 | 60.00 |
| ATOM | 2221 | N | THR | 546 | 35.013 | -6.003 | 100.138 | 1.00 | 60.00 |
| ATOM | 2223 | CA | THR | 546 | 34.063 | -4.943 | 100.276 | 1.00 | 60.00 |
| ATOM | 2224 | CB | THR | 546 | 32.913 | -5.316 | 101.162 | 1.00 | 60.00 |
| ATOM | 2225 | OG1 | THR | 546 | 32.278 | -6.482 | 100.657 | 1.00 | 60.00 |
| ATOM | 2227 | CG2 | THR | 546 | 31.908 | -4.155 | 101.168 | 1.00 | 60.00 |
| ATOM | 2228 | C | THR | 546 | 34.655 | -3.679 | 100.798 | 1.00 | 60.00 |
| ATOM | 2229 | O | THR | 546 | 35.273 | -3.653 | 101.862 | 1.00 | 60.00 |
| ATOM | 2230 | N | CYS | 547 | 34.478 | -2.587 | 100.028 | 1.00 | 20.00 |
| ATOM | 2232 | CA | CYS | 547 | 34.910 | -1.291 | 100.451 | 1.00 | 20.00 |
| ATOM | 2233 | CB | CYS | 547 | 36.397 | -0.993 | 100.138 | 1.00 | 20.00 |
| ATOM | 2234 | SG | CYS | 547 | 36.804 | -0.821 | 98.370 | 1.00 | 20.00 |
| ATOM | 2235 | C | CYS | 547 | 34.054 | -0.301 | 99.741 | 1.00 | 20.00 |
| ATOM | 2236 | O | CYS | 547 | 33.714 | -0.488 | 98.574 | 1.00 | 20.00 |
| ATOM | 2237 | N | THR | 548 | 33.658 | 0.777 | 100.443 | 1.00 | 20.00 |
| ATOM | 2239 | CA | THR | 548 | 32.823 | 1.753 | 99.812 | 1.00 | 20.00 |
| ATOM | 2240 | CB | THR | 548 | 32.286 | 2.785 | 100.761 | 1.00 | 20.00 |
| ATOM | 2241 | OG1 | THR | 548 | 31.326 | 3.597 | 100.100 | 1.00 | 20.00 |
| ATOM | 2243 | CG2 | THR | 548 | 33.444 | 3.643 | 101.295 | 1.00 | 20.00 |
| ATOM | 2244 | C | THR | 548 | 33.588 | 2.446 | 98.731 | 1.00 | 20.00 |
| ATOM | 2245 | O | THR | 548 | 33.071 | 2.659 | 97.635 | 1.00 | 20.00 |
| ATOM | 2246 | N | GLY | 549 | 34.860 | 2.795 | 99.006 | 1.00 | 20.00 |
| ATOM | 2248 | CA | GLY | 549 | 35.646 | 3.490 | 98.029 | 1.00 | 20.00 |
| ATOM | 2249 | C | GLY | 549 | 37.075 | 3.158 | 98.301 | 1.00 | 20.00 |
| ATOM | 2250 | O | GLY | 549 | 37.389 | 2.474 | 99.273 | 1.00 | 20.00 |
| ATOM | 2251 | N | ARG | 550 | 37.987 | 3.642 | 97.439 | 1.00 | 40.00 |
| ATOM | 2253 | CA | ARG | 550 | 39.369 | 3.329 | 97.635 | 1.00 | 40.00 |
| ATOM | 2254 | CB | ARG | 550 | 40.252 | 3.660 | 96.418 | 1.00 | 40.00 |
| ATOM | 2255 | CG | ARG | 550 | 40.302 | 5.146 | 96.055 | 1.00 | 40.00 |
| ATOM | 2256 | CD | ARG | 550 | 40.796 | 5.399 | 94.628 | 1.00 | 40.00 |
| ATOM | 2257 | NE | ARG | 550 | 41.174 | 6.836 | 94.522 | 1.00 | 40.00 |
| ATOM | 2259 | CZ | ARG | 550 | 42.474 | 7.204 | 94.715 | 1.00 | 40.00 |
| ATOM | 2260 | NH1 | ARG | 550 | 43.427 | 6.249 | 94.930 | 1.00 | 40.00 |
| ATOM | 2263 | NH2 | ARG | 550 | 42.824 | 8.522 | 94.685 | 1.00 | 40.00 |
| ATOM | 2266 | C | ARG | 550 | 39.863 | 4.106 | 98.812 | 1.00 | 40.00 |
| ATOM | 2267 | O | ARG | 550 | 39.578 | 5.294 | 98.953 | 1.00 | 40.00 |
| ATOM | 2268 | N | GLY | 551 | 40.613 | 3.430 | 99.704 | 1.00 | 40.00 |
| ATOM | 2270 | CA | GLY | 551 | 41.142 | 4.071 | 100.872 | 1.00 | 40.00 |
| ATOM | 2271 | C | GLY | 551 | 40.981 | 3.097 | 101.997 | 1.00 | 40.00 |
| ATOM | 2272 | O | GLY | 551 | 40.006 | 2.350 | 102.054 | 1.00 | 40.00 |
| ATOM | 2273 | N | PRO | 552 | 41.932 | 3.085 | 102.888 | 1.00 | 20.00 |
| ATOM | 2274 | CD | PRO | 552 | 43.306 | 3.313 | 102.469 | 1.00 | 20.00 |
| ATOM | 2275 | CA | PRO | 552 | 41.863 | 2.176 | 104.002 | 1.00 | 20.00 |
| ATOM | 2276 | CB | PRO | 552 | 43.276 | 2.098 | 104.570 | 1.00 | 20.00 |
| ATOM | 2277 | CG | PRO | 552 | 44.168 | 2.400 | 103.355 | 1.00 | 20.00 |
| ATOM | 2278 | C | PRO | 552 | 40.827 | 2.555 | 105.015 | 1.00 | 20.00 |
| ATOM | 2279 | O | PRO | 552 | 40.513 | 1.735 | 105.877 | 1.00 | 20.00 |
| ATOM | 2280 | N | ASP | 553 | 40.354 | 3.812 | 104.987 | 1.00 | 20.00 |
| ATOM | 2282 | CA | ASP | 553 | 39.319 | 4.262 | 105.875 | 1.00 | 20.00 |
| ATOM | 2283 | CB | ASP | 553 | 39.206 | 5.796 | 105.947 | 1.00 | 20.00 |
| ATOM | 2284 | CG | ASP | 553 | 38.294 | 6.152 | 107.117 | 1.00 | 20.00 |
| ATOM | 2285 | OD1 | ASP | 553 | 37.963 | 7.359 | 107.264 | 1.00 | 20.00 |
| ATOM | 2286 | OD2 | ASP | 553 | 37.920 | 5.225 | 107.883 | 1.00 | 20.00 |
| ATOM | 2287 | C | ASP | 553 | 37.996 | 3.743 | 105.403 | 1.00 | 20.00 |
| ATOM | 2288 | O | ASP | 553 | 37.059 | 3.556 | 106.176 | 1.00 | 20.00 |
| ATOM | 2289 | N | ASN | 554 | 37.896 | 3.535 | 104.081 | 1.00 | 20.00 |
| ATOM | 2291 | CA | ASN | 554 | 36.688 | 3.161 | 103.405 | 1.00 | 20.00 |
| ATOM | 2292 | CB | ASN | 554 | 36.819 | 3.236 | 101.872 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2293 | CG | ASN | 554 | 36.906 | 4.697 | 101.440 | 1.00 | 20.00 |
| ATOM | 2294 | OD1 | ASN | 554 | 36.433 | 5.049 | 100.361 | 1.00 | 20.00 |
| ATOM | 2295 | ND2 | ASN | 554 | 37.526 | 5.567 | 102.283 | 1.00 | 20.00 |
| ATOM | 2298 | C | ASN | 554 | 36.198 | 1.788 | 103.736 | 1.00 | 20.00 |
| ATOM | 2299 | O | ASN | 554 | 35.006 | 1.510 | 103.612 | 1.00 | 20.00 |
| ATOM | 2300 | N | CYS | 555 | 37.096 | 0.882 | 104.155 | 1.00 | 20.00 |
| ATOM | 2302 | CA | CYS | 555 | 36.709 | -0.487 | 104.278 | 1.00 | 20.00 |
| ATOM | 2303 | CB | CYS | 555 | 37.838 | -1.410 | 104.693 | 1.00 | 20.00 |
| ATOM | 2304 | SG | CYS | 555 | 37.418 | -3.035 | 104.055 | 1.00 | 20.00 |
| ATOM | 2305 | C | CYS | 555 | 35.503 | -0.772 | 105.127 | 1.00 | 20.00 |
| ATOM | 2306 | O | CYS | 555 | 35.108 | 0.013 | 105.987 | 1.00 | 20.00 |
| ATOM | 2307 | N | ILE | 556 | 34.806 | -1.877 | 104.783 | 1.00 | 20.00 |
| ATOM | 2309 | CA | ILE | 556 | 33.694 | -2.389 | 105.529 | 1.00 | 20.00 |
| ATOM | 2310 | CB | ILE | 556 | 32.844 | -3.320 | 104.721 | 1.00 | 20.00 |
| ATOM | 2311 | CG2 | ILE | 556 | 31.910 | -4.052 | 105.694 | 1.00 | 20.00 |
| ATOM | 2312 | CG1 | ILE | 556 | 32.088 | -2.530 | 103.635 | 1.00 | 20.00 |
| ATOM | 2313 | CD1 | ILE | 556 | 32.991 | -1.832 | 102.621 | 1.00 | 20.00 |
| ATOM | 2314 | C | ILE | 556 | 34.192 | -3.107 | 106.749 | 1.00 | 20.00 |
| ATOM | 2315 | O | ILE | 556 | 33.569 | -3.044 | 107.807 | 1.00 | 20.00 |
| ATOM | 2316 | N | GLN | 557 | 35.331 | -3.827 | 106.620 | 1.00 | 20.00 |
| ATOM | 2318 | CA | GLN | 557 | 35.888 | -4.574 | 107.717 | 1.00 | 20.00 |
| ATOM | 2319 | CB | GLN | 557 | 35.398 | -6.031 | 107.749 | 1.00 | 20.00 |
| ATOM | 2320 | CG | GLN | 557 | 35.950 | -6.848 | 108.917 | 1.00 | 20.00 |
| ATOM | 2321 | CD | GLN | 557 | 35.315 | -6.317 | 110.194 | 1.00 | 20.00 |
| ATOM | 2322 | OE1 | GLN | 557 | 35.729 | -5.293 | 110.735 | 1.00 | 20.00 |
| ATOM | 2323 | NE2 | GLN | 557 | 34.271 | -7.033 | 110.688 | 1.00 | 20.00 |
| ATOM | 2326 | C | GLN | 557 | 37.382 | -4.600 | 107.564 | 1.00 | 20.00 |
| ATOM | 2327 | O | GLN | 557 | 37.912 | -4.188 | 106.540 | 1.00 | 20.00 |
| ATOM | 2328 | N | CYS | 558 | 38.134 | -5.090 | 108.568 | 1.00 | 20.00 |
| ATOM | 2330 | CA | CYS | 558 | 39.559 | -5.011 | 108.413 | 1.00 | 20.00 |
| ATOM | 2331 | CB | CYS | 558 | 40.210 | -4.242 | 109.577 | 1.00 | 20.00 |
| ATOM | 2332 | SG | CYS | 558 | 41.972 | -3.888 | 109.346 | 1.00 | 20.00 |
| ATOM | 2333 | C | CYS | 558 | 40.134 | -6.394 | 108.333 | 1.00 | 20.00 |
| ATOM | 2334 | O | CYS | 558 | 39.608 | -7.331 | 108.930 | 1.00 | 20.00 |
| ATOM | 2335 | N | ALA | 559 | 41.202 | -6.562 | 107.523 | 1.00 | 20.00 |
| ATOM | 2337 | CA | ALA | 559 | 41.859 | -7.831 | 107.368 | 1.00 | 20.00 |
| ATOM | 2338 | CB | ALA | 559 | 42.906 | -7.830 | 106.242 | 1.00 | 20.00 |
| ATOM | 2339 | C | ALA | 559 | 42.574 | -8.172 | 108.632 | 1.00 | 20.00 |
| ATOM | 2340 | O | ALA | 559 | 42.555 | -9.314 | 109.090 | 1.00 | 20.00 |
| ATOM | 2341 | N | HIS | 560 | 43.214 | -7.155 | 109.234 | 1.00 | 20.00 |
| ATOM | 2343 | CA | HIS | 560 | 44.004 | -7.333 | 110.413 | 1.00 | 20.00 |
| ATOM | 2344 | CB | HIS | 560 | 45.392 | -6.679 | 110.300 | 1.00 | 20.00 |
| ATOM | 2345 | CG | HIS | 560 | 46.258 | -7.335 | 109.265 | 1.00 | 20.00 |
| ATOM | 2346 | CD2 | HIS | 560 | 47.279 | -8.222 | 109.413 | 1.00 | 20.00 |
| ATOM | 2347 | ND1 | HIS | 560 | 46.127 | -7.137 | 107.907 | 1.00 | 20.00 |
| ATOM | 2349 | CE1 | HIS | 560 | 47.068 | -7.908 | 107.307 | 1.00 | 20.00 |
| ATOM | 2350 | NE2 | HIS | 560 | 47.792 | -8.585 | 108.180 | 1.00 | 20.00 |
| ATOM | 2352 | C | HIS | 560 | 43.278 | -6.659 | 111.530 | 1.00 | 20.00 |
| ATOM | 2353 | O | HIS | 560 | 42.187 | -7.077 | 111.915 | 1.00 | 20.00 |
| ATOM | 2354 | N | TYR | 561 | 43.886 | -5.602 | 112.101 | 1.00 | 20.00 |
| ATOM | 2356 | CA | TYR | 561 | 43.280 | -4.944 | 113.218 | 1.00 | 20.00 |
| ATOM | 2357 | CB | TYR | 561 | 44.253 | -4.731 | 114.387 | 1.00 | 20.00 |
| ATOM | 2358 | CG | TYR | 561 | 44.768 | -6.077 | 114.759 | 1.00 | 20.00 |
| ATOM | 2359 | CD1 | TYR | 561 | 45.838 | -6.609 | 114.078 | 1.00 | 20.00 |
| ATOM | 2360 | CE1 | TYR | 561 | 46.328 | -7.852 | 114.398 | 1.00 | 20.00 |
| ATOM | 2361 | CD2 | TYR | 561 | 44.182 | -6.812 | 115.764 | 1.00 | 20.00 |
| ATOM | 2362 | CE2 | TYR | 561 | 44.670 | -8.055 | 116.091 | 1.00 | 20.00 |
| ATOM | 2363 | CZ | TYR | 561 | 45.744 | -8.576 | 115.408 | 1.00 | 20.00 |
| ATOM | 2364 | OH | TYR | 561 | 46.253 | -9.847 | 115.746 | 1.00 | 20.00 |
| ATOM | 2366 | C | TYR | 561 | 42.788 | -3.592 | 112.823 | 1.00 | 20.00 |
| ATOM | 2367 | O | TYR | 561 | 43.405 | -2.896 | 112.019 | 1.00 | 20.00 |
| ATOM | 2368 | N | ILE | 562 | 41.644 | -3.183 | 113.406 | 1.00 | 20.00 |
| ATOM | 2370 | CA | ILE | 562 | 41.077 | -1.904 | 113.085 | 1.00 | 20.00 |
| ATOM | 2371 | CB | ILE | 562 | 39.577 | -1.918 | 113.043 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2372 | CG2 | ILE | 562 | 39.101 | -0.478 | 112.787 | 1.00 | 20.00 |
| ATOM | 2373 | CG1 | ILE | 562 | 39.067 | -2.929 | 112.004 | 1.00 | 20.00 |
| ATOM | 2374 | CD1 | ILE | 562 | 37.575 | -3.238 | 112.135 | 1.00 | 20.00 |
| ATOM | 2375 | C | ILE | 562 | 41.455 | -0.963 | 114.180 | 1.00 | 20.00 |
| ATOM | 2376 | O | ILE | 562 | 41.281 | -1.264 | 115.360 | 1.00 | 20.00 |
| ATOM | 2377 | N | ASP | 563 | 42.010 | 0.207 | 113.817 | 1.00 | 20.00 |
| ATOM | 2379 | CA | ASP | 563 | 42.386 | 1.150 | 114.825 | 1.00 | 20.00 |
| ATOM | 2380 | CB | ASP | 563 | 43.880 | 1.091 | 115.205 | 1.00 | 20.00 |
| ATOM | 2381 | CG | ASP | 563 | 44.724 | 1.403 | 113.981 | 1.00 | 20.00 |
| ATOM | 2382 | OD1 | ASP | 563 | 44.203 | 1.239 | 112.847 | 1.00 | 20.00 |
| ATOM | 2383 | OD2 | ASP | 563 | 45.905 | 1.802 | 114.161 | 1.00 | 20.00 |
| ATOM | 2384 | C | ASP | 563 | 42.058 | 2.534 | 114.384 | 1.00 | 20.00 |
| ATOM | 2385 | O | ASP | 563 | 42.380 | 2.940 | 113.269 | 1.00 | 20.00 |
| ATOM | 2386 | N | GLY | 564 | 41.419 | 3.312 | 115.279 | 1.00 | 20.00 |
| ATOM | 2388 | CA | GLY | 564 | 40.994 | 4.620 | 114.891 | 1.00 | 20.00 |
| ATOM | 2389 | C | GLY | 564 | 40.076 | 4.323 | 113.755 | 1.00 | 20.00 |
| ATOM | 2390 | O | GLY | 564 | 39.370 | 3.320 | 113.749 | 1.00 | 20.00 |
| ATOM | 2391 | N | PRO | 565 | 40.053 | 5.164 | 112.786 | 1.00 | 20.00 |
| ATOM | 2392 | CD | PRO | 565 | 39.999 | 6.582 | 113.110 | 1.00 | 20.00 |
| ATOM | 2393 | CA | PRO | 565 | 39.193 | 4.835 | 111.684 | 1.00 | 20.00 |
| ATOM | 2394 | CB | PRO | 565 | 38.720 | 6.167 | 111.103 | 1.00 | 20.00 |
| ATOM | 2395 | CG | PRO | 565 | 38.849 | 7.155 | 112.272 | 1.00 | 20.00 |
| ATOM | 2396 | C | PRO | 565 | 39.914 | 4.021 | 110.669 | 1.00 | 20.00 |
| ATOM | 2397 | O | PRO | 565 | 39.330 | 3.776 | 109.616 | 1.00 | 20.00 |
| ATOM | 2398 | N | HIS | 566 | 41.161 | 3.590 | 110.938 | 1.00 | 20.00 |
| ATOM | 2400 | CA | HIS | 566 | 41.857 | 2.923 | 109.880 | 1.00 | 20.00 |
| ATOM | 2401 | CB | HIS | 566 | 43.245 | 3.513 | 109.586 | 1.00 | 20.00 |
| ATOM | 2402 | CG | HIS | 566 | 43.183 | 4.857 | 108.927 | 1.00 | 20.00 |
| ATOM | 2403 | CD2 | HIS | 566 | 42.946 | 5.175 | 107.625 | 1.00 | 20.00 |
| ATOM | 2404 | ND1 | HIS | 566 | 43.342 | 6.056 | 109.584 | 1.00 | 20.00 |
| ATOM | 2406 | CE1 | HIS | 566 | 43.198 | 7.033 | 108.654 | 1.00 | 20.00 |
| ATOM | 2407 | NE2 | HIS | 566 | 42.955 | 6.547 | 107.449 | 1.00 | 20.00 |
| ATOM | 2409 | C | HIS | 566 | 42.052 | 1.463 | 110.093 | 1.00 | 20.00 |
| ATOM | 2410 | O | HIS | 566 | 42.131 | 0.968 | 111.216 | 1.00 | 20.00 |
| ATOM | 2411 | N | CYS | 567 | 42.132 | 0.741 | 108.961 | 1.00 | 20.00 |
| ATOM | 2413 | CA | CYS | 567 | 42.335 | -0.671 | 108.965 | 1.00 | 20.00 |
| ATOM | 2414 | CB | CYS | 567 | 41.714 | -1.325 | 107.712 | 1.00 | 20.00 |
| ATOM | 2415 | SG | CYS | 567 | 42.066 | -3.090 | 107.483 | 1.00 | 20.00 |
| ATOM | 2416 | C | CYS | 567 | 43.819 | -0.844 | 108.966 | 1.00 | 20.00 |
| ATOM | 2417 | O | CYS | 567 | 44.481 | -0.582 | 107.963 | 1.00 | 20.00 |
| ATOM | 2418 | N | VAL | 568 | 44.384 | -1.275 | 110.117 | 1.00 | 20.00 |
| ATOM | 2420 | CA | VAL | 568 | 45.807 | -1.419 | 110.192 | 1.00 | 20.00 |
| ATOM | 2421 | CB | VAL | 568 | 46.459 | -0.634 | 111.294 | 1.00 | 20.00 |
| ATOM | 2422 | CG1 | VAL | 568 | 47.967 | -0.920 | 111.276 | 1.00 | 20.00 |
| ATOM | 2423 | CG2 | VAL | 568 | 46.188 | 0.853 | 111.019 | 1.00 | 20.00 |
| ATOM | 2424 | C | VAL | 568 | 46.191 | -2.866 | 110.262 | 1.00 | 20.00 |
| ATOM | 2425 | O | VAL | 568 | 45.432 | -3.715 | 110.728 | 1.00 | 20.00 |
| ATOM | 2426 | N | LYS | 569 | 47.374 | -3.176 | 109.694 | 1.00 | 20.00 |
| ATOM | 2428 | CA | LYS | 569 | 47.951 | -4.488 | 109.640 | 1.00 | 20.00 |
| ATOM | 2429 | CB | LYS | 569 | 49.216 | -4.537 | 108.767 | 1.00 | 20.00 |
| ATOM | 2430 | CG | LYS | 569 | 50.380 | -3.748 | 109.372 | 1.00 | 20.00 |
| ATOM | 2431 | CD | LYS | 569 | 51.739 | -4.059 | 108.741 | 1.00 | 20.00 |
| ATOM | 2432 | CE | LYS | 569 | 51.942 | -3.404 | 107.375 | 1.00 | 20.00 |
| ATOM | 2433 | NZ | LYS | 569 | 53.302 | -3.698 | 106.869 | 1.00 | 20.00 |
| ATOM | 2437 | C | LYS | 569 | 48.373 | -4.943 | 111.002 | 1.00 | 20.00 |
| ATOM | 2438 | O | LYS | 569 | 48.320 | -6.133 | 111.312 | 1.00 | 20.00 |
| ATOM | 2439 | N | THR | 570 | 48.869 | -4.007 | 111.834 | 1.00 | 20.00 |
| ATOM | 2441 | CA | THR | 570 | 49.301 | -4.370 | 113.153 | 1.00 | 20.00 |
| ATOM | 2442 | CB | THR | 570 | 50.768 | -4.685 | 113.237 | 1.00 | 20.00 |
| ATOM | 2443 | OG1 | THR | 570 | 51.085 | -5.252 | 114.500 | 1.00 | 20.00 |
| ATOM | 2445 | CG2 | THR | 570 | 51.560 | -3.385 | 113.022 | 1.00 | 20.00 |
| ATOM | 2446 | C | THR | 570 | 49.043 | -3.196 | 114.041 | 1.00 | 20.00 |
| ATOM | 2447 | O | THR | 570 | 48.887 | -2.073 | 113.571 | 1.00 | 20.00 |
| ATOM | 2448 | N | CYS | 571 | 49.001 | -3.415 | 115.365 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2450 | CA | CYS | 571 | 48.677 | -2.326 | 116.236 | 1.00 | 20.00 |
| ATOM | 2451 | CB | CYS | 571 | 48.297 | -2.778 | 117.655 | 1.00 | 20.00 |
| ATOM | 2452 | SG | CYS | 571 | 46.798 | -3.800 | 117.635 | 1.00 | 20.00 |
| ATOM | 2453 | C | CYS | 571 | 49.804 | -1.347 | 116.339 | 1.00 | 20.00 |
| ATOM | 2454 | O | CYS | 571 | 50.985 | -1.688 | 116.291 | 1.00 | 20.00 |
| ATOM | 2455 | N | PRO | 572 | 49.410 | -0.109 | 116.467 | 1.00 | 20.00 |
| ATOM | 2456 | CD | PRO | 572 | 48.187 | 0.334 | 115.816 | 1.00 | 20.00 |
| ATOM | 2457 | CA | PRO | 572 | 50.361 | 0.959 | 116.601 | 1.00 | 20.00 |
| ATOM | 2458 | CB | PRO | 572 | 49.585 | 2.247 | 116.339 | 1.00 | 20.00 |
| ATOM | 2459 | CG | PRO | 572 | 48.435 | 1.798 | 115.422 | 1.00 | 20.00 |
| ATOM | 2460 | C | PRO | 572 | 50.958 | 0.895 | 117.971 | 1.00 | 20.00 |
| ATOM | 2461 | O | PRO | 572 | 50.380 | 0.244 | 118.840 | 1.00 | 20.00 |
| ATOM | 2462 | N | ALA | 573 | 52.112 | 1.553 | 118.188 | 1.00 | 20.00 |
| ATOM | 2464 | CA | ALA | 573 | 52.753 | 1.489 | 119.469 | 1.00 | 20.00 |
| ATOM | 2465 | CB | ALA | 573 | 54.133 | 2.167 | 119.501 | 1.00 | 20.00 |
| ATOM | 2466 | C | ALA | 573 | 51.895 | 2.147 | 120.503 | 1.00 | 20.00 |
| ATOM | 2467 | O | ALA | 573 | 51.194 | 3.120 | 120.229 | 1.00 | 20.00 |
| ATOM | 2468 | N | GLY | 574 | 51.916 | 1.586 | 121.729 | 1.00 | 20.00 |
| ATOM | 2470 | CA | GLY | 574 | 51.186 | 2.136 | 122.834 | 1.00 | 20.00 |
| ATOM | 2471 | C | GLY | 574 | 49.808 | 1.556 | 122.845 | 1.00 | 20.00 |
| ATOM | 2472 | O | GLY | 574 | 49.070 | 1.709 | 123.817 | 1.00 | 20.00 |
| ATOM | 2473 | N | VAL | 575 | 49.425 | 0.868 | 121.753 | 1.00 | 20.00 |
| ATOM | 2475 | CA | VAL | 575 | 48.121 | 0.274 | 121.693 | 1.00 | 20.00 |
| ATOM | 2476 | CB | VAL | 575 | 47.314 | 0.725 | 120.509 | 1.00 | 20.00 |
| ATOM | 2477 | CG1 | VAL | 575 | 46.002 | -0.078 | 120.470 | 1.00 | 20.00 |
| ATOM | 2478 | CG2 | VAL | 575 | 47.105 | 2.245 | 120.612 | 1.00 | 20.00 |
| ATOM | 2479 | C | VAL | 575 | 48.343 | -1.194 | 121.542 | 1.00 | 20.00 |
| ATOM | 2480 | O | VAL | 575 | 49.335 | -1.621 | 120.954 | 1.00 | 20.00 |
| ATOM | 2481 | N | MET | 576 | 47.427 | -2.014 | 122.094 | 1.00 | 20.00 |
| ATOM | 2483 | CA | MET | 576 | 47.607 | -3.428 | 121.978 | 1.00 | 20.00 |
| ATOM | 2484 | CB | MET | 576 | 47.818 | -4.162 | 123.311 | 1.00 | 20.00 |
| ATOM | 2485 | CG | MET | 576 | 48.045 | -5.662 | 123.110 | 1.00 | 20.00 |
| ATOM | 2486 | SD | MET | 576 | 49.614 | -6.061 | 122.282 | 1.00 | 20.00 |
| ATOM | 2487 | CE | MET | 576 | 49.204 | -7.800 | 121.961 | 1.00 | 20.00 |
| ATOM | 2488 | C | MET | 576 | 46.416 | -4.041 | 121.335 | 1.00 | 20.00 |
| ATOM | 2489 | O | MET | 576 | 45.309 | -3.507 | 121.390 | 1.00 | 20.00 |
| ATOM | 2490 | N | GLY | 577 | 46.635 | -5.196 | 120.684 | 1.00 | 20.00 |
| ATOM | 2492 | CA | GLY | 577 | 45.556 | -5.868 | 120.037 | 1.00 | 20.00 |
| ATOM | 2493 | C | GLY | 577 | 44.786 | -6.565 | 121.098 | 1.00 | 20.00 |
| ATOM | 2494 | O | GLY | 577 | 45.342 | -7.317 | 121.898 | 1.00 | 20.00 |
| ATOM | 2495 | N | GLU | 578 | 43.466 | -6.324 | 121.130 | 1.00 | 40.00 |
| ATOM | 2497 | CA | GLU | 578 | 42.669 | -6.989 | 122.105 | 1.00 | 40.00 |
| ATOM | 2498 | CB | GLU | 578 | 41.196 | -6.551 | 122.069 | 1.00 | 40.00 |
| ATOM | 2499 | CG | GLU | 578 | 40.554 | -6.705 | 120.691 | 1.00 | 40.00 |
| ATOM | 2500 | CD | GLU | 578 | 39.200 | -6.015 | 120.734 | 1.00 | 40.00 |
| ATOM | 2501 | OE1 | GLU | 578 | 38.692 | -5.780 | 121.862 | 1.00 | 40.00 |
| ATOM | 2502 | OE2 | GLU | 578 | 38.658 | -5.709 | 119.638 | 1.00 | 40.00 |
| ATOM | 2503 | C | GLU | 578 | 42.767 | -8.436 | 121.768 | 1.00 | 40.00 |
| ATOM | 2504 | O | GLU | 578 | 42.470 | -8.837 | 120.643 | 1.00 | 40.00 |
| ATOM | 2505 | N | ASN | 579 | 43.221 | -9.250 | 122.741 | 1.00 | 40.00 |
| ATOM | 2507 | CA | ASN | 579 | 43.379 | -10.652 | 122.497 | 1.00 | 40.00 |
| ATOM | 2508 | CB | ASN | 579 | 43.876 | -11.428 | 123.731 | 1.00 | 40.00 |
| ATOM | 2509 | CG | ASN | 579 | 45.318 | -11.027 | 124.006 | 1.00 | 40.00 |
| ATOM | 2510 | OD1 | ASN | 579 | 45.789 | -11.102 | 125.141 | 1.00 | 40.00 |
| ATOM | 2511 | ND2 | ASN | 579 | 46.041 | -10.587 | 122.942 | 1.00 | 40.00 |
| ATOM | 2514 | C | ASN | 579 | 42.032 | -11.186 | 122.157 | 1.00 | 40.00 |
| ATOM | 2515 | O | ASN | 579 | 41.839 | -11.805 | 121.113 | 1.00 | 40.00 |
| ATOM | 2516 | N | ASN | 580 | 41.051 | -10.939 | 123.042 | 1.00 | 60.00 |
| ATOM | 2518 | CA | ASN | 580 | 39.724 | -11.401 | 122.781 | 1.00 | 60.00 |
| ATOM | 2519 | CB | ASN | 580 | 39.352 | -12.684 | 123.545 | 1.00 | 60.00 |
| ATOM | 2520 | CG | ASN | 580 | 40.171 | -13.837 | 122.979 | 1.00 | 60.00 |
| ATOM | 2521 | OD1 | ASN | 580 | 40.127 | -14.129 | 121.785 | 1.00 | 60.00 |
| ATOM | 2522 | ND2 | ASN | 580 | 40.949 | -14.516 | 123.865 | 1.00 | 60.00 |
| ATOM | 2525 | C | ASN | 580 | 38.812 | -10.328 | 123.263 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2526 | O | ASN | 580 | 39.232 | -9.411 | 123.968 | 1.00 | 60.00 |
| ATOM | 2527 | N | THR | 581 | 37.530 | -10.406 | 122.869 | 1.00 | 60.00 |
| ATOM | 2529 | CA | THR | 581 | 36.598 | -9.428 | 123.333 | 1.00 | 60.00 |
| i 4 | 2530 | CB | THR | 581 | 35.565 | -9.040 | 122.316 | 1.00 | 60.00 |
| ATOM | 2531 | OG1 | THR | 581 | 36.188 | -8.483 | 121.168 | 1.00 | 60.00 |
| ATOM | 2533 | CG2 | THR | 581 | 34.606 | -8.019 | 122.953 | 1.00 | 60.00 |
| ATOM | 2534 | C | THR | 581 | 35.871 | -10.061 | 124.467 | 1.00 | 60.00 |
| ATOM | 2535 | O | THR | 581 | 35.253 | -11.113 | 124.311 | 1.00 | 60.00 |
| ATOM | 2536 | N | LEU | 582 | 35.949 | -9.440 | 125.656 | 1.00 | 60.00 |
| ATOM | 2538 | CA | LEU | 582 | 35.234 | -9.983 | 126.768 | 1.00 | 60.00 |
| ATOM | 2539 | CB | LEU | 582 | 35.778 | -9.531 | 128.134 | 1.00 | 60.00 |
| ATOM | 2540 | CG | LEU | 582 | 35.012 | -10.111 | 129.338 | 1.00 | 60.00 |
| ATOM | 2541 | CD1 | LEU | 582 | 35.132 | -11.644 | 129.400 | 1.00 | 60.00 |
| ATOM | 2542 | CD2 | LEU | 582 | 35.449 | -9.427 | 130.643 | 1.00 | 60.00 |
| ATOM | 2543 | C | LEU | 582 | 33.850 | -9.457 | 126.615 | 1.00 | 60.00 |
| ATOM | 2544 | O | LEU | 582 | 33.652 | -8.300 | 126.247 | 1.00 | 60.00 |
| ATOM | 2545 | N | VAL | 583 | 32.841 | -10.305 | 126.882 | 1.00 | 60.00 |
| ATOM | 2547 | CA | VAL | 583 | 31.499 | -9.852 | 126.695 | 1.00 | 60.00 |
| ATOM | 2548 | CB | VAL | 583 | 30.462 | -10.907 | 126.944 | 1.00 | 60.00 |
| ATOM | 2549 | CG1 | VAL | 583 | 29.073 | -10.265 | 126.789 | 1.00 | 60.00 |
| ATOM | 2550 | CG2 | VAL | 583 | 30.715 | -12.079 | 125.980 | 1.00 | 60.00 |
| ATOM | 2551 | C | VAL | 583 | 31.241 | -8.720 | 127.629 | 1.00 | 60.00 |
| ATOM | 2552 | O | VAL | 583 | 31.685 | -8.722 | 128.776 | 1.00 | 60.00 |
| ATOM | 2553 | N | TRP | 584 | 30.519 | -7.702 | 127.128 | 1.00 | 60.00 |
| ATOM | 2555 | CA | TRP | 584 | 30.185 | -6.554 | 127.914 | 1.00 | 60.00 |
| ATOM | 2556 | CB | TRP | 584 | 31.011 | -5.309 | 127.545 | 1.00 | 60.00 |
| ATOM | 2557 | CG | TRP | 584 | 30.852 | -4.141 | 128.493 | 1.00 | 60.00 |
| ATOM | 2558 | CD2 | TRP | 584 | 31.646 | -2.948 | 128.430 | 1.00 | 60.00 |
| ATOM | 2559 | CE2 | TRP | 584 | 31.259 | -2.139 | 129.496 | 1.00 | 60.00 |
| ATOM | 2560 | CE3 | TRP | 584 | 32.627 | -2.561 | 127.561 | 1.00 | 60.00 |
| ATOM | 2561 | CD1 | TRP | 584 | 30.038 | -4.008 | 129.578 | 1.00 | 60.00 |
| ATOM | 2562 | NE1 | TRP | 584 | 30.266 | -2.799 | 130.191 | 1.00 | 60.00 |
| ATOM | 2564 | CZ2 | TRP | 584 | 31.844 | -0.923 | 129.710 | 1.00 | 60.00 |
| ATOM | 2565 | CZ3 | TRP | 584 | 33.218 | -1.337 | 127.780 | 1.00 | 60.00 |
| ATOM | 2566 | CH2 | TRP | 584 | 32.833 | -0.533 | 128.833 | 1.00 | 60.00 |
| ATOM | 2567 | C | TRP | 584 | 28.765 | -6.301 | 127.534 | 1.00 | 60.00 |
| ATOM | 2568 | O | TRP | 584 | 28.044 | -7.238 | 127.193 | 1.00 | 60.00 |
| ATOM | 2569 | N | LYS | 585 | 28.305 | -5.038 | 127.602 | 1.00 | 60.00 |
| ATOM | 2571 | CA | LYS | 585 | 26.959 | -4.800 | 127.178 | 1.00 | 60.00 |
| ATOM | 2572 | CB | LYS | 585 | 26.533 | -3.325 | 127.263 | 1.00 | 60.00 |
| ATOM | 2573 | CG | LYS | 585 | 26.441 | -2.801 | 128.696 | 1.00 | 60.00 |
| ATOM | 2574 | CD | LYS | 585 | 26.260 | -1.285 | 128.778 | 1.00 | 60.00 |
| ATOM | 2575 | CE | LYS | 585 | 27.256 | -0.509 | 127.914 | 1.00 | 60.00 |
| ATOM | 2576 | NZ | LYS | 585 | 28.639 | -0.882 | 128.280 | 1.00 | 60.00 |
| ATOM | 2580 | C | LYS | 585 | 26.950 | -5.188 | 125.739 | 1.00 | 60.00 |
| ATOM | 2581 | O | LYS | 585 | 26.086 | -5.936 | 125.287 | 1.00 | 60.00 |
| ATOM | 2582 | N | TYR | 586 | 27.950 | -4.691 | 124.988 | 1.00 | 60.00 |
| ATOM | 2584 | CA | TYR | 586 | 28.085 | -5.043 | 123.609 | 1.00 | 60.00 |
| ATOM | 2585 | CB | TYR | 586 | 27.690 | -3.915 | 122.638 | 1.00 | 60.00 |
| ATOM | 2586 | CG | TYR | 586 | 28.454 | -2.688 | 122.991 | 1.00 | 60.00 |
| ATOM | 2587 | CD1 | TYR | 586 | 29.742 | -2.502 | 122.545 | 1.00 | 60.00 |
| ATOM | 2588 | CE1 | TYR | 586 | 30.421 | -1.346 | 122.848 | 1.00 | 60.00 |
| ATOM | 2589 | CD2 | TYR | 586 | 27.853 | -1.698 | 123.734 | 1.00 | 60.00 |
| ATOM | 2590 | CE2 | TYR | 586 | 28.527 | -0.541 | 124.039 | 1.00 | 60.00 |
| ATOM | 2591 | CZ | TYR | 586 | 29.814 | -0.364 | 123.594 | 1.00 | 60.00 |
| ATOM | 2592 | OH | TYR | 586 | 30.511 | 0.821 | 123.910 | 1.00 | 60.00 |
| ATOM | 2594 | C | TYR | 586 | 29.514 | -5.422 | 123.390 | 1.00 | 60.00 |
| ATOM | 2595 | O | TYR | 586 | 30.384 | -5.086 | 124.192 | 1.00 | 60.00 |
| ATOM | 2596 | N | ALA | 587 | 29.789 | -6.164 | 122.299 | 1.00 | 60.00 |
| ATOM | 2598 | CA | ALA | 587 | 31.126 | -6.622 | 122.057 | 1.00 | 60.00 |
| ATOM | 2599 | CB | ALA | 587 | 31.191 | -8.068 | 121.539 | 1.00 | 60.00 |
| ATOM | 2600 | C | ALA | 587 | 31.792 | -5.762 | 121.035 | 1.00 | 60.00 |
| ATOM | 2601 | O | ALA | 587 | 31.219 | -4.793 | 120.541 | 1.00 | 60.00 |
| ATOM | 2602 | N | ASP | 588 | 33.053 | -6.109 | 120.713 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2604 | CA | ASP | 588 | 33.809 | -5.378 | 119.742 | 1.00 | 60.00 |
| ATOM | 2605 | CB | ASP | 588 | 35.298 | -5.256 | 120.109 | 1.00 | 60.00 |
| ATOM | 2606 | CG | ASP | 588 | 35.393 | -4.378 | 121.349 | 1.00 | 60.00 |
| ATOM | 2607 | OD1 | ASP | 588 | 34.698 | -3.327 | 121.383 | 1.00 | 60.00 |
| ATOM | 2608 | OD2 | ASP | 588 | 36.148 | -4.754 | 122.286 | 1.00 | 60.00 |
| ATOM | 2609 | C | ASP | 588 | 33.720 | -6.146 | 118.465 | 1.00 | 60.00 |
| ATOM | 2610 | O | ASP | 588 | 33.563 | -7.366 | 118.473 | 1.00 | 60.00 |
| ATOM | 2611 | N | ALA | 589 | 33.802 | -5.442 | 117.320 | 1.00 | 60.00 |
| ATOM | 2613 | CA | ALA | 589 | 33.704 | -6.126 | 116.067 | 1.00 | 60.00 |
| ATOM | 2614 | CB | ALA | 589 | 32.786 | -5.424 | 115.050 | 1.00 | 60.00 |
| ATOM | 2615 | C | ALA | 589 | 35.061 | -6.195 | 115.453 | 1.00 | 60.00 |
| ATOM | 2616 | O | ALA | 589 | 35.884 | -5.296 | 115.622 | 1.00 | 60.00 |
| ATOM | 2617 | N | GLY | 590 | 35.329 | -7.298 | 114.730 | 1.00 | 60.00 |
| ATOM | 2619 | CA | GLY | 590 | 36.583 | -7.458 | 114.058 | 1.00 | 60.00 |
| ATOM | 2620 | C | GLY | 590 | 37.680 | -7.372 | 115.064 | 1.00 | 60.00 |
| ATOM | 2621 | O | GLY | 590 | 37.439 | -7.336 | 116.269 | 1.00 | 60.00 |
| ATOM | 2622 | N | HIS | 591 | 38.932 | -7.335 | 114.574 | 1.00 | 60.00 |
| ATOM | 2624 | CA | HIS | 591 | 40.055 | -7.246 | 115.456 | 1.00 | 60.00 |
| ATOM | 2625 | CB | HIS | 591 | 41.328 | -7.879 | 114.871 | 1.00 | 60.00 |
| ATOM | 2626 | CG | HIS | 591 | 41.115 | -9.292 | 114.411 | 1.00 | 60.00 |
| ATOM | 2627 | CD2 | HIS | 591 | 40.894 | -9.768 | 113.156 | 1.00 | 60.00 |
| ATOM | 2628 | ND1 | HIS | 591 | 41.088 | -10.392 | 115.240 | 1.00 | 60.00 |
| ATOM | 2630 | CE1 | HIS | 591 | 40.855 | -11.471 | 114.449 | 1.00 | 60.00 |
| ATOM | 2631 | NE2 | HIS | 591 | 40.731 | -11.142 | 113.176 | 1.00 | 60.00 |
| ATOM | 2633 | C | HIS | 591 | 40.311 | -5.785 | 115.616 | 1.00 | 60.00 |
| ATOM | 2634 | O | HIS | 591 | 40.255 | -5.028 | 114.649 | 1.00 | 60.00 |
| ATOM | 2635 | N | VAL | 592 | 40.576 | -5.339 | 116.859 | 1.00 | 40.00 |
| ATOM | 2637 | CA | VAL | 592 | 40.795 | -3.939 | 117.059 | 1.00 | 40.00 |
| ATOM | 2638 | CB | VAL | 592 | 39.588 | -3.239 | 117.628 | 1.00 | 40.00 |
| ATOM | 2639 | CG1 | VAL | 592 | 39.887 | -1.741 | 117.821 | 1.00 | 40.00 |
| ATOM | 2640 | CG2 | VAL | 592 | 38.401 | -3.505 | 116.688 | 1.00 | 40.00 |
| ATOM | 2641 | C | VAL | 592 | 41.929 | -3.781 | 118.019 | 1.00 | 40.00 |
| ATOM | 2642 | O | VAL | 592 | 42.264 | -4.696 | 118.769 | 1.00 | 40.00 |
| ATOM | 2643 | N | CYS | 593 | 42.565 | -2.597 | 117.989 | 1.00 | 20.00 |
| ATOM | 2645 | CA | CYS | 593 | 43.667 | -2.310 | 118.848 | 1.00 | 20.00 |
| ATOM | 2646 | CB | CYS | 593 | 44.810 | -1.588 | 118.120 | 1.00 | 20.00 |
| ATOM | 2647 | SG | CYS | 593 | 45.453 | -2.575 | 116.742 | 1.00 | 20.00 |
| ATOM | 2648 | C | CYS | 593 | 43.150 | -1.376 | 119.893 | 1.00 | 20.00 |
| ATOM | 2649 | O | CYS | 593 | 42.462 | -0.405 | 119.583 | 1.00 | 20.00 |
| ATOM | 2650 | N | HIS | 594 | 43.460 | -1.661 | 121.173 | 1.00 | 20.00 |
| ATOM | 2652 | CA | HIS | 594 | 42.998 | -0.809 | 122.227 | 1.00 | 20.00 |
| ATOM | 2653 | CB | HIS | 594 | 42.101 | -1.511 | 123.263 | 1.00 | 20.00 |
| ATOM | 2654 | CG | HIS | 594 | 40.743 | -1.878 | 122.739 | 1.00 | 20.00 |
| ATOM | 2655 | CD2 | HIS | 594 | 40.271 | -3.063 | 122.262 | 1.00 | 20.00 |
| ATOM | 2656 | ND1 | HIS | 594 | 39.677 | -1.007 | 122.698 | 1.00 | 20.00 |
| ATOM | 2658 | CE1 | HIS | 594 | 38.622 | -1.700 | 122.200 | 1.00 | 20.00 |
| ATOM | 2659 | NE2 | HIS | 594 | 38.935 | -2.953 | 121.920 | 1.00 | 20.00 |
| ATOM | 2661 | C | HIS | 594 | 44.178 | -0.267 | 122.972 | 1.00 | 20.00 |
| ATOM | 2662 | O | HIS | 594 | 45.251 | -0.867 | 122.987 | 1.00 | 20.00 |
| ATOM | 2663 | N | LEU | 595 | 43.994 | 0.898 | 123.625 | 1.00 | 20.00 |
| ATOM | 2665 | CA | LEU | 595 | 45.068 | 1.563 | 124.306 | 1.00 | 20.00 |
| ATOM | 2666 | CB | LEU | 595 | 44.724 | 3.014 | 124.684 | 1.00 | 20.00 |
| ATOM | 2667 | CG | LEU | 595 | 45.878 | 3.792 | 125.340 | 1.00 | 20.00 |
| ATOM | 2668 | CD1 | LEU | 595 | 47.067 | 3.945 | 124.376 | 1.00 | 20.00 |
| ATOM | 2669 | CD2 | LEU | 595 | 45.390 | 5.145 | 125.882 | 1.00 | 20.00 |
| ATOM | 2670 | C | LEU | 595 | 45.454 | 0.813 | 125.533 | 1.00 | 20.00 |
| ATOM | 2671 | O | LEU | 595 | 44.630 | 0.164 | 126.176 | 1.00 | 20.00 |
| ATOM | 2672 | N | CYS | 596 | 46.758 | 0.870 | 125.863 | 1.00 | 20.00 |
| ATOM | 2674 | CA | CYS | 596 | 47.264 | 0.207 | 127.023 | 1.00 | 20.00 |
| ATOM | 2675 | CB | CYS | 596 | 48.515 | -0.637 | 126.706 | 1.00 | 20.00 |
| ATOM | 2676 | SG | CYS | 596 | 49.102 | -1.717 | 128.046 | 1.00 | 20.00 |
| ATOM | 2677 | C | CYS | 596 | 47.623 | 1.323 | 127.945 | 1.00 | 20.00 |
| ATOM | 2678 | O | CYS | 596 | 48.193 | 2.327 | 127.521 | 1.00 | 20.00 |
| ATOM | 2679 | N | HIS | 597 | 47.271 | 1.201 | 129.238 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|--------|---------|------|-------|
| ATOM | 2681 | CA | HIS | 597 | 47.588 | 2.296 | 130.103 | 1.00 | 20.00 |
| ATOM | 2682 | CB | HIS | 597 | 47.048 | 2.169 | 131.538 | 1.00 | 20.00 |
| ATOM | 2683 | CG | HIS | 597 | 47.173 | 3.456 | 132.300 | 1.00 | 20.00 |
| i 4 | 2684 | CD2 | HIS | 597 | 46.290 | 4.484 | 132.432 | 1.00 | 20.00 |
| ATOM | 2685 | ND1 | HIS | 597 | 48.302 | 3.843 | 132.988 | 1.00 | 20.00 |
| ATOM | 2687 | CE1 | HIS | 597 | 48.046 | 5.072 | 133.502 | 1.00 | 20.00 |
| ATOM | 2688 | NE2 | HIS | 597 | 46.837 | 5.503 | 133.190 | 1.00 | 20.00 |
| ATOM | 2690 | C | HIS | 597 | 49.072 | 2.360 | 130.162 | 1.00 | 20.00 |
| ATOM | 2691 | O | HIS | 597 | 49.764 | 1.360 | 129.977 | 1.00 | 20.00 |
| ATOM | 2692 | N | PRO | 598 | 49.579 | 3.531 | 130.393 | 1.00 | 20.00 |
| ATOM | 2693 | CD | PRO | 598 | 48.912 | 4.745 | 129.963 | 1.00 | 20.00 |
| ATOM | 2694 | CA | PRO | 598 | 51.001 | 3.693 | 130.432 | 1.00 | 20.00 |
| ATOM | 2695 | CB | PRO | 598 | 51.263 | 5.199 | 130.329 | 1.00 | 20.00 |
| ATOM | 2696 | CG | PRO | 598 | 49.870 | 5.853 | 130.423 | 1.00 | 20.00 |
| ATOM | 2697 | C | PRO | 598 | 51.602 | 3.024 | 131.623 | 1.00 | 20.00 |
| ATOM | 2698 | O | PRO | 598 | 52.811 | 2.794 | 131.617 | 1.00 | 20.00 |
| ATOM | 2699 | N | ASN | 599 | 50.801 | 2.740 | 132.668 | 1.00 | 20.00 |
| ATOM | 2701 | CA | ASN | 599 | 51.344 | 2.085 | 133.822 | 1.00 | 20.00 |
| ATOM | 2702 | CB | ASN | 599 | 50.402 | 2.076 | 135.045 | 1.00 | 20.00 |
| ATOM | 2703 | CG | ASN | 599 | 49.235 | 1.134 | 134.789 | 1.00 | 20.00 |
| ATOM | 2704 | OD1 | ASN | 599 | 48.184 | 1.517 | 134.280 | 1.00 | 20.00 |
| ATOM | 2705 | ND2 | ASN | 599 | 49.442 | -0.161 | 135.149 | 1.00 | 20.00 |
| ATOM | 2708 | C | ASN | 599 | 51.666 | 0.659 | 133.500 | 1.00 | 20.00 |
| ATOM | 2709 | O | ASN | 599 | 52.704 | 0.136 | 133.906 | 1.00 | 20.00 |
| ATOM | 2710 | N | CYS | 600 | 50.788 | -0.012 | 132.731 | 1.00 | 20.00 |
| ATOM | 2712 | CA | CYS | 600 | 50.992 | -1.409 | 132.501 | 1.00 | 20.00 |
| ATOM | 2713 | CB | CYS | 600 | 49.842 | -2.099 | 131.762 | 1.00 | 20.00 |
| ATOM | 2714 | SG | CYS | 600 | 50.052 | -3.899 | 131.760 | 1.00 | 20.00 |
| ATOM | 2715 | C | CYS | 600 | 52.221 | -1.614 | 131.694 | 1.00 | 20.00 |
| ATOM | 2716 | O | CYS | 600 | 52.686 | -0.712 | 130.998 | 1.00 | 20.00 |
| ATOM | 2717 | N | THR | 601 | 52.793 | -2.827 | 131.802 | 1.00 | 20.00 |
| ATOM | 2719 | CA | THR | 601 | 53.970 | -3.148 | 131.063 | 1.00 | 20.00 |
| ATOM | 2720 | CB | THR | 601 | 55.171 | -3.395 | 131.927 | 1.00 | 20.00 |
| ATOM | 2721 | OG1 | THR | 601 | 56.342 | -3.487 | 131.129 | 1.00 | 20.00 |
| ATOM | 2723 | CG2 | THR | 601 | 54.952 | -4.707 | 132.700 | 1.00 | 20.00 |
| ATOM | 2724 | C | THR | 601 | 53.703 | -4.418 | 130.327 | 1.00 | 20.00 |
| ATOM | 2725 | O | THR | 601 | 52.841 | -5.208 | 130.709 | 1.00 | 20.00 |
| ATOM | 2726 | N | TYR | 602 | 54.441 | -4.621 | 129.223 | 1.00 | 20.00 |
| ATOM | 2728 | CA | TYR | 602 | 54.362 | -5.817 | 128.443 | 1.00 | 20.00 |
| ATOM | 2729 | CB | TYR | 602 | 54.867 | -7.057 | 129.202 | 1.00 | 20.00 |
| ATOM | 2730 | CG | TYR | 602 | 56.329 | -6.858 | 129.410 | 1.00 | 20.00 |
| ATOM | 2731 | CD1 | TYR | 602 | 56.796 | -6.184 | 130.515 | 1.00 | 20.00 |
| ATOM | 2732 | CE1 | TYR | 602 | 58.142 | -5.949 | 130.676 | 1.00 | 20.00 |
| ATOM | 2733 | CD2 | TYR | 602 | 57.227 | -7.268 | 128.452 | 1.00 | 20.00 |
| ATOM | 2734 | CE2 | TYR | 602 | 58.573 | -7.031 | 128.605 | 1.00 | 20.00 |
| ATOM | 2735 | CZ | TYR | 602 | 59.034 | -6.373 | 129.720 | 1.00 | 20.00 |
| ATOM | 2736 | OH | TYR | 602 | 60.414 | -6.121 | 129.872 | 1.00 | 20.00 |
| ATOM | 2738 | C | TYR | 602 | 53.006 | -6.118 | 127.884 | 1.00 | 20.00 |
| ATOM | 2739 | O | TYR | 602 | 52.663 | -7.285 | 127.710 | 1.00 | 20.00 |
| ATOM | 2740 | N | GLY | 603 | 52.193 | -5.088 | 127.573 | 1.00 | 20.00 |
| ATOM | 2742 | CA | GLY | 603 | 50.950 | -5.364 | 126.904 | 1.00 | 20.00 |
| ATOM | 2743 | C | GLY | 603 | 49.741 | -5.200 | 127.771 | 1.00 | 20.00 |
| ATOM | 2744 | O | GLY | 603 | 49.831 | -5.132 | 128.996 | 1.00 | 20.00 |
| ATOM | 2745 | N | CYS | 604 | 48.564 | -5.116 | 127.110 | 1.00 | 20.00 |
| ATOM | 2747 | CA | CYS | 604 | 47.299 | -5.006 | 127.778 | 1.00 | 20.00 |
| ATOM | 2748 | CB | CYS | 604 | 46.694 | -3.589 | 127.763 | 1.00 | 20.00 |
| ATOM | 2749 | SG | CYS | 604 | 47.402 | -2.388 | 128.930 | 1.00 | 20.00 |
| ATOM | 2750 | C | CYS | 604 | 46.311 | -5.849 | 127.031 | 1.00 | 20.00 |
| ATOM | 2751 | O | CYS | 604 | 46.297 | -5.866 | 125.800 | 1.00 | 20.00 |
| ATOM | 2752 | N | THR | 605 | 45.467 | -6.601 | 127.765 | 1.00 | 20.00 |
| ATOM | 2754 | CA | THR | 605 | 44.432 | -7.348 | 127.116 | 1.00 | 20.00 |
| ATOM | 2755 | CB | THR | 605 | 43.712 | -8.300 | 128.033 | 1.00 | 20.00 |
| ATOM | 2756 | OG1 | THR | 605 | 42.795 | -9.093 | 127.292 | 1.00 | 20.00 |
| ATOM | 2758 | CG2 | THR | 605 | 42.979 | -7.508 | 129.129 | 1.00 | 20.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2759 | C | THR | 605 | 43.453 | -6.350 | 126.590 | 1.00 | 20.00 |
| ATOM | 2760 | O | THR | 605 | 42.937 | -6.487 | 125.482 | 1.00 | 20.00 |
| ATOM | 2761 | N | GLY | 606 | 43.191 | -5.295 | 127.388 | 1.00 | 20.00 |
| ATOM | 2763 | CA | GLY | 606 | 42.260 | -4.280 | 126.998 | 1.00 | 20.00 |
| ATOM | 2764 | C | GLY | 606 | 42.606 | -3.041 | 127.757 | 1.00 | 20.00 |
| ATOM | 2765 | O | GLY | 606 | 43.364 | -3.061 | 128.725 | 1.00 | 20.00 |
| ATOM | 2766 | N | PRO | 607 | 42.027 | -1.958 | 127.325 | 1.00 | 40.00 |
| ATOM | 2767 | CD | PRO | 607 | 40.706 | -2.007 | 126.719 | 1.00 | 40.00 |
| ATOM | 2768 | CA | PRO | 607 | 42.301 | -0.674 | 127.908 | 1.00 | 40.00 |
| ATOM | 2769 | CB | PRO | 607 | 41.315 | 0.279 | 127.244 | 1.00 | 40.00 |
| ATOM | 2770 | CG | PRO | 607 | 40.092 | -0.622 | 126.987 | 1.00 | 40.00 |
| ATOM | 2771 | C | PRO | 607 | 42.024 | -0.743 | 129.374 | 1.00 | 40.00 |
| ATOM | 2772 | O | PRO | 607 | 41.162 | -1.522 | 129.776 | 1.00 | 40.00 |
| ATOM | 2773 | N | GLY | 608 | 42.749 | 0.046 | 130.191 | 1.00 | 40.00 |
| ATOM | 2775 | CA | GLY | 608 | 42.462 | 0.063 | 131.595 | 1.00 | 40.00 |
| ATOM | 2776 | C | GLY | 608 | 43.620 | -0.455 | 132.383 | 1.00 | 40.00 |
| ATOM | 2777 | O | GLY | 608 | 44.459 | -1.200 | 131.881 | 1.00 | 40.00 |
| ATOM | 2778 | N | LEU | 609 | 43.675 | -0.047 | 133.666 | 1.00 | 20.00 |
| ATOM | 2780 | CA | LEU | 609 | 44.685 | -0.468 | 134.593 | 1.00 | 20.00 |
| ATOM | 2781 | CB | LEU | 609 | 44.536 | 0.218 | 135.962 | 1.00 | 20.00 |
| ATOM | 2782 | CG | LEU | 609 | 45.581 | -0.222 | 137.005 | 1.00 | 20.00 |
| ATOM | 2783 | CD1 | LEU | 609 | 47.002 | 0.209 | 136.609 | 1.00 | 20.00 |
| ATOM | 2784 | CD2 | LEU | 609 | 45.180 | 0.238 | 138.415 | 1.00 | 20.00 |
| ATOM | 2785 | C | LEU | 609 | 44.529 | -1.936 | 134.820 | 1.00 | 20.00 |
| ATOM | 2786 | O | LEU | 609 | 45.510 | -2.671 | 134.926 | 1.00 | 20.00 |
| ATOM | 2787 | N | GLU | 610 | 43.268 | -2.394 | 134.896 | 1.00 | 20.00 |
| ATOM | 2789 | CA | GLU | 610 | 42.951 | -3.768 | 135.153 | 1.00 | 20.00 |
| ATOM | 2790 | CB | GLU | 610 | 41.439 | -4.034 | 135.267 | 1.00 | 20.00 |
| ATOM | 2791 | CG | GLU | 610 | 40.784 | -3.454 | 136.522 | 1.00 | 20.00 |
| ATOM | 2792 | CD | GLU | 610 | 40.474 | -1.986 | 136.274 | 1.00 | 20.00 |
| ATOM | 2793 | OE1 | GLU | 610 | 40.013 | -1.657 | 135.149 | 1.00 | 20.00 |
| ATOM | 2794 | OE2 | GLU | 610 | 40.693 | -1.174 | 137.212 | 1.00 | 20.00 |
| ATOM | 2795 | C | GLU | 610 | 43.449 | -4.617 | 134.033 | 1.00 | 20.00 |
| ATOM | 2796 | O | GLU | 610 | 43.861 | -5.757 | 134.241 | 1.00 | 20.00 |
| ATOM | 2797 | N | GLY | 611 | 43.438 | -4.066 | 132.809 | 1.00 | 20.00 |
| ATOM | 2799 | CA | GLY | 611 | 43.816 | -4.811 | 131.648 | 1.00 | 20.00 |
| ATOM | 2800 | C | GLY | 611 | 45.192 | -5.340 | 131.856 | 1.00 | 20.00 |
| ATOM | 2801 | O | GLY | 611 | 45.560 | -6.368 | 131.291 | 1.00 | 20.00 |
| ATOM | 2802 | N | CYS | 612 | 46.004 | -4.617 | 132.648 | 1.00 | 20.00 |
| ATOM | 2804 | CA | CYS | 612 | 47.344 | -5.054 | 132.897 | 1.00 | 20.00 |
| ATOM | 2805 | CB | CYS | 612 | 48.076 | -4.190 | 133.927 | 1.00 | 20.00 |
| ATOM | 2806 | SG | CYS | 612 | 49.864 | -4.351 | 133.729 | 1.00 | 20.00 |
| ATOM | 2807 | C | CYS | 612 | 47.272 | -6.451 | 133.421 | 1.00 | 20.00 |
| ATOM | 2808 | O | CYS | 612 | 46.224 | -6.915 | 133.873 | 1.00 | 20.00 |
| ATOM | 2809 | N | PRO | 613 | 48.373 | -7.149 | 133.341 | 1.00 | 60.00 |
| ATOM | 2810 | CD | PRO | 613 | 49.228 | -6.991 | 132.183 | 1.00 | 60.00 |
| ATOM | 2811 | CA | PRO | 613 | 48.378 | -8.500 | 133.834 | 1.00 | 60.00 |
| ATOM | 2812 | CB | PRO | 613 | 49.563 | -9.188 | 133.157 | 1.00 | 60.00 |
| ATOM | 2813 | CG | PRO | 613 | 49.734 | -8.405 | 131.846 | 1.00 | 60.00 |
| ATOM | 2814 | C | PRO | 613 | 48.448 | -8.547 | 135.319 | 1.00 | 60.00 |
| ATOM | 2815 | O | PRO | 613 | 48.851 | -7.567 | 135.934 | 1.00 | 60.00 |
| ATOM | 2816 | N | THR | 614 | 48.042 | -9.690 | 135.912 | 1.00 | 60.00 |
| ATOM | 2818 | CA | THR | 614 | 48.080 | -9.856 | 137.334 | 1.00 | 60.00 |
| ATOM | 2819 | CB | THR | 614 | 46.716 | -9.892 | 137.960 | 1.00 | 60.00 |
| ATOM | 2820 | OG1 | THR | 614 | 46.814 | -9.809 | 139.377 | 1.00 | 60.00 |
| ATOM | 2822 | CG2 | THR | 614 | 46.026 | -11.203 | 137.550 | 1.00 | 60.00 |
| ATOM | 2823 | C | THR | 614 | 48.711 | -11.188 | 137.572 | 1.00 | 60.00 |
| ATOM | 2824 | O | THR | 614 | 49.329 | -11.761 | 136.676 | 1.00 | 60.00 |
| ATOM | 2825 | N | ASN | 615 | 48.591 | -11.704 | 138.810 | 1.00 | 60.00 |
| ATOM | 2827 | CA | ASN | 615 | 49.141 | -12.989 | 139.110 | 1.00 | 60.00 |
| ATOM | 2828 | CB | ASN | 615 | 48.878 | -13.439 | 140.557 | 1.00 | 60.00 |
| ATOM | 2829 | CG | ASN | 615 | 49.650 | -12.521 | 141.491 | 1.00 | 60.00 |
| ATOM | 2830 | OD1 | ASN | 615 | 49.126 | -12.068 | 142.508 | 1.00 | 60.00 |
| ATOM | 2831 | ND2 | ASN | 615 | 50.933 | -12.237 | 141.141 | 1.00 | 60.00 |

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|------|------|-----|-----|-----|--------|---------|---------|------|-------|
| ATOM | 2834 | C | ASN | 615 | 48.428 | -13.952 | 138.225 | 1.00 | 60.00 |
| ATOM | 2835 | O | ASN | 615 | 49.035 | -14.838 | 137.625 | 1.00 | 60.00 |
| ATOM | 2836 | N | GLY | 616 | 47.099 | -13.780 | 138.110 | 1.00 | 60.00 |
| ATOM | 2838 | CA | GLY | 616 | 46.324 | -14.672 | 137.308 | 1.00 | 60.00 |
| ATOM | 2839 | C | GLY | 616 | 45.593 | -15.544 | 138.269 | 1.00 | 60.00 |
| ATOM | 2840 | O | GLY | 616 | 45.794 | -15.467 | 139.480 | 1.00 | 60.00 |
| ATOM | 2841 | N | PRO | 617 | 44.734 | -16.368 | 137.747 | 1.00 | 60.00 |
| ATOM | 2842 | CD | PRO | 617 | 43.932 | -15.954 | 136.607 | 1.00 | 60.00 |
| ATOM | 2843 | CA | PRO | 617 | 44.008 | -17.246 | 138.618 | 1.00 | 60.00 |
| ATOM | 2844 | CB | PRO | 617 | 42.801 | -17.730 | 137.819 | 1.00 | 60.00 |
| ATOM | 2845 | CG | PRO | 617 | 42.545 | -16.582 | 136.827 | 1.00 | 60.00 |
| ATOM | 2846 | C | PRO | 617 | 44.910 | -18.336 | 139.081 | 1.00 | 60.00 |
| ATOM | 2847 | O | PRO | 617 | 45.878 | -18.646 | 138.387 | 1.00 | 60.00 |
| ATOM | 2848 | N | LYS | 618 | 44.622 | -18.921 | 140.257 | 1.00 | 60.00 |
| ATOM | 2850 | CA | LYS | 618 | 45.463 | -19.964 | 140.754 | 1.00 | 60.00 |
| ATOM | 2851 | CB | LYS | 618 | 44.979 | -20.535 | 142.097 | 1.00 | 60.00 |
| ATOM | 2852 | CG | LYS | 618 | 44.979 | -19.536 | 143.255 | 1.00 | 60.00 |
| ATOM | 2853 | CD | LYS | 618 | 44.189 | -20.044 | 144.463 | 1.00 | 60.00 |
| ATOM | 2854 | CE | LYS | 618 | 42.726 | -20.355 | 144.136 | 1.00 | 60.00 |
| ATOM | 2855 | NZ | LYS | 618 | 42.066 | -20.995 | 145.296 | 1.00 | 60.00 |
| ATOM | 2859 | C | LYS | 618 | 45.382 | -21.073 | 139.764 | 1.00 | 60.00 |
| ATOM | 2860 | O | LYS | 618 | 46.397 | -21.621 | 139.338 | 1.00 | 60.00 |
| ATOM | 2861 | N | ILE | 619 | 44.147 | -21.416 | 139.355 | 1.00 | 60.00 |
| ATOM | 2863 | CA | ILE | 619 | 43.985 | -22.494 | 138.432 | 1.00 | 60.00 |
| ATOM | 2864 | CB | ILE | 619 | 42.708 | -23.256 | 138.630 | 1.00 | 60.00 |
| ATOM | 2865 | CG2 | ILE | 619 | 42.592 | -24.284 | 137.493 | 1.00 | 60.00 |
| ATOM | 2866 | CG1 | ILE | 619 | 42.667 | -23.878 | 140.036 | 1.00 | 60.00 |
| ATOM | 2867 | CD1 | ILE | 619 | 43.798 | -24.870 | 140.301 | 1.00 | 60.00 |
| ATOM | 2868 | C | ILE | 619 | 43.939 | -21.931 | 137.055 | 1.00 | 60.00 |
| ATOM | 2869 | O | ILE | 619 | 42.903 | -21.468 | 136.579 | 1.00 | 60.00 |
| ATOM | 2870 | N | PRO | 620 | 45.064 | -21.962 | 136.408 | 1.00 | 60.00 |
| ATOM | 2871 | CD | PRO | 620 | 46.133 | -22.886 | 136.747 | 1.00 | 60.00 |
| ATOM | 2872 | CA | PRO | 620 | 45.150 | -21.499 | 135.056 | 1.00 | 60.00 |
| ATOM | 2873 | CB | PRO | 620 | 46.580 | -21.807 | 134.621 | 1.00 | 60.00 |
| ATOM | 2874 | CG | PRO | 620 | 46.929 | -23.064 | 135.443 | 1.00 | 60.00 |
| ATOM | 2875 | C | PRO | 620 | 44.167 | -22.326 | 134.296 | 1.00 | 60.00 |
| ATOM | 2876 | O | PRO | 620 | 43.890 | -23.448 | 134.719 | 1.00 | 60.00 |
| ATOM | 2877 | N | SER | 621 | 43.605 | -21.796 | 133.195 | 1.00 | 60.00 |
| ATOM | 2879 | CA | SER | 621 | 42.673 | -22.575 | 132.437 | 1.00 | 60.00 |
| ATOM | 2880 | CB | SER | 621 | 41.697 | -21.723 | 131.609 | 1.00 | 60.00 |
| ATOM | 2881 | OG | SER | 621 | 40.848 | -20.982 | 132.473 | 1.00 | 60.00 |
| ATOM | 2883 | C | SER | 621 | 43.486 | -23.423 | 131.466 | 1.00 | 60.00 |
| ATOM | 2884 | O | SER | 621 | 44.310 | -22.836 | 130.715 | 1.00 | 60.00 |
| ATOM | 2885 | OXT | SER | 621 | 43.293 | -24.669 | 131.461 | 1.00 | 60.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 240 | N | LEU | 25 | 50.889 | 2.127 | 50.184 | 1.00 | 40.00 |
| ATOM | 242 | CA | LEU | 25 | 52.244 | 2.155 | 50.646 | 1.00 | 40.00 |
| ATOM | 243 | CB | LEU | 25 | 53.260 | 1.846 | 49.534 | 1.00 | 40.00 |
| ATOM | 244 | CG | LEU | 25 | 53.122 | 0.432 | 48.944 | 1.00 | 40.00 |
| ATOM | 245 | CD1 | LEU | 25 | 51.761 | 0.244 | 48.255 | 1.00 | 40.00 |
| ATOM | 246 | CD2 | LEU | 25 | 54.305 | 0.103 | 48.021 | 1.00 | 40.00 |
| ATOM | 247 | C | LEU | 25 | 52.535 | 3.540 | 51.127 | 1.00 | 40.00 |
| ATOM | 248 | O | LEU | 25 | 53.309 | 3.726 | 52.063 | 1.00 | 40.00 |
| ATOM | 249 | N | SER | 26 | 51.919 | 4.552 | 50.489 | 1.00 | 40.00 |
| ATOM | 251 | CA | SER | 26 | 52.128 | 5.925 | 50.853 | 1.00 | 40.00 |
| ATOM | 252 | CB | SER | 26 | 51.479 | 6.924 | 49.885 | 1.00 | 40.00 |
| ATOM | 253 | OG | SER | 26 | 52.186 | 6.916 | 48.654 | 1.00 | 40.00 |
| ATOM | 255 | C | SER | 26 | 51.646 | 6.179 | 52.249 | 1.00 | 40.00 |
| ATOM | 256 | O | SER | 26 | 52.061 | 7.144 | 52.888 | 1.00 | 40.00 |
| ATOM | 257 | N | LEU | 27 | 50.743 | 5.316 | 52.751 | 1.00 | 40.00 |
| ATOM | 259 | CA | LEU | 27 | 50.199 | 5.423 | 54.077 | 1.00 | 40.00 |
| ATOM | 260 | CB | LEU | 27 | 49.203 | 4.300 | 54.426 | 1.00 | 40.00 |
| ATOM | 261 | CG | LEU | 27 | 47.799 | 4.468 | 53.815 | 1.00 | 40.00 |
| ATOM | 262 | CD1 | LEU | 27 | 47.097 | 5.687 | 54.425 | 1.00 | 40.00 |
| ATOM | 263 | CD2 | LEU | 27 | 47.820 | 4.503 | 52.280 | 1.00 | 40.00 |
| ATOM | 264 | C | LEU | 27 | 51.282 | 5.372 | 55.114 | 1.00 | 40.00 |
| ATOM | 265 | O | LEU | 27 | 51.125 | 5.920 | 56.202 | 1.00 | 40.00 |
| ATOM | 266 | N | GLN | 28 | 52.404 | 4.695 | 54.814 | 1.00 | 40.00 |
| ATOM | 268 | CA | GLN | 28 | 53.475 | 4.531 | 55.757 | 1.00 | 40.00 |
| ATOM | 269 | CB | GLN | 28 | 54.656 | 3.726 | 55.191 | 1.00 | 40.00 |
| ATOM | 270 | CG | GLN | 28 | 55.794 | 3.551 | 56.199 | 1.00 | 40.00 |
| ATOM | 271 | CD | GLN | 28 | 56.903 | 2.750 | 55.531 | 1.00 | 40.00 |
| ATOM | 272 | OE1 | GLN | 28 | 57.466 | 3.169 | 54.524 | 1.00 | 40.00 |
| ATOM | 273 | NE2 | GLN | 28 | 57.222 | 1.561 | 56.110 | 1.00 | 40.00 |
| ATOM | 276 | C | GLN | 28 | 54.028 | 5.843 | 56.214 | 1.00 | 40.00 |
| ATOM | 277 | O | GLN | 28 | 54.444 | 5.978 | 57.363 | 1.00 | 40.00 |
| ATOM | 278 | N | ARG | 29 | 54.025 | 6.858 | 55.334 | 1.00 | 40.00 |
| ATOM | 280 | CA | ARG | 29 | 54.608 | 8.130 | 55.649 | 1.00 | 40.00 |
| ATOM | 281 | CB | ARG | 29 | 54.373 | 9.157 | 54.531 | 1.00 | 40.00 |
| ATOM | 282 | CG | ARG | 29 | 54.975 | 10.528 | 54.816 | 1.00 | 40.00 |
| ATOM | 283 | CD | ARG | 29 | 54.807 | 11.506 | 53.653 | 1.00 | 40.00 |
| ATOM | 284 | NE | ARG | 29 | 55.608 | 10.980 | 52.511 | 1.00 | 40.00 |
| ATOM | 286 | CZ | ARG | 29 | 55.054 | 10.093 | 51.634 | 1.00 | 40.00 |
| ATOM | 287 | NH1 | ARG | 29 | 53.754 | 9.702 | 51.785 | 1.00 | 40.00 |
| ATOM | 290 | NH2 | ARG | 29 | 55.800 | 9.597 | 50.603 | 1.00 | 40.00 |
| ATOM | 293 | C | ARG | 29 | 53.987 | 8.647 | 56.906 | 1.00 | 40.00 |
| ATOM | 294 | O | ARG | 29 | 54.629 | 9.325 | 57.707 | 1.00 | 40.00 |
| ATOM | 295 | N | MET | 30 | 52.697 | 8.347 | 57.100 | 1.00 | 40.00 |
| ATOM | 297 | CA | MET | 30 | 51.985 | 8.770 | 58.264 | 1.00 | 40.00 |
| ATOM | 298 | CB | MET | 30 | 50.510 | 8.341 | 58.207 | 1.00 | 40.00 |
| ATOM | 299 | CG | MET | 30 | 49.715 | 8.969 | 57.061 | 1.00 | 40.00 |
| ATOM | 300 | SD | MET | 30 | 49.219 | 10.693 | 57.345 | 1.00 | 40.00 |
| ATOM | 301 | CE | MET | 30 | 47.920 | 10.259 | 58.538 | 1.00 | 40.00 |
| ATOM | 302 | C | MET | 30 | 52.545 | 8.139 | 59.503 | 1.00 | 40.00 |
| ATOM | 303 | O | MET | 30 | 52.717 | 8.798 | 60.525 | 1.00 | 40.00 |
| ATOM | 304 | N | PHE | 31 | 52.864 | 6.835 | 59.432 | 1.00 | 40.00 |
| ATOM | 306 | CA | PHE | 31 | 53.208 | 6.092 | 60.610 | 1.00 | 40.00 |
| ATOM | 307 | CB | PHE | 31 | 53.368 | 4.587 | 60.332 | 1.00 | 40.00 |
| ATOM | 308 | CG | PHE | 31 | 53.702 | 3.932 | 61.628 | 1.00 | 40.00 |
| ATOM | 309 | CD1 | PHE | 31 | 52.704 | 3.584 | 62.509 | 1.00 | 40.00 |
| ATOM | 310 | CD2 | PHE | 31 | 55.009 | 3.671 | 61.966 | 1.00 | 40.00 |
| ATOM | 311 | CE1 | PHE | 31 | 53.005 | 2.991 | 63.712 | 1.00 | 40.00 |
| ATOM | 312 | CE2 | PHE | 31 | 55.316 | 3.078 | 63.169 | 1.00 | 40.00 |
| ATOM | 313 | CZ | PHE | 31 | 54.313 | 2.738 | 64.045 | 1.00 | 40.00 |
| ATOM | 314 | C | PHE | 31 | 54.443 | 6.531 | 61.331 | 1.00 | 40.00 |
| ATOM | 315 | O | PHE | 31 | 54.430 | 6.668 | 62.553 | 1.00 | 40.00 |
| ATOM | 316 | N | ASN | 32 | 55.545 | 6.784 | 60.607 | 1.00 | 40.00 |
| ATOM | 318 | CA | ASN | 32 | 56.765 | 7.029 | 61.316 | 1.00 | 40.00 |
| ATOM | 319 | CB | ASN | 32 | 57.986 | 7.127 | 60.383 | 1.00 | 40.00 |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 320 | CG | ASN | 32 | 57.792 | 8.311 | 59.452 | 1.00 | 40.00 |
| ATOM | 321 | OD1 | ASN | 32 | 56.702 | 8.526 | 58.926 | 1.00 | 40.00 |
| ATOM | 322 | ND2 | ASN | 32 | 58.877 | 9.105 | 59.244 | 1.00 | 40.00 |
| VM | 325 | C | ASN | 32 | 56.761 | 8.237 | 62.192 | 1.00 | 40.00 |
| ATOM | 326 | O | ASN | 32 | 57.023 | 8.132 | 63.389 | 1.00 | 40.00 |
| ATOM | 327 | N | ASN | 33 | 56.425 | 9.425 | 61.661 | 1.00 | 40.00 |
| ATOM | 329 | CA | ASN | 33 | 56.577 | 10.527 | 62.559 | 1.00 | 40.00 |
| ATOM | 330 | CB | ASN | 33 | 57.776 | 11.425 | 62.207 | 1.00 | 40.00 |
| ATOM | 331 | CG | ASN | 33 | 59.052 | 10.651 | 62.509 | 1.00 | 40.00 |
| ATOM | 332 | OD1 | ASN | 33 | 59.275 | 10.223 | 63.640 | 1.00 | 40.00 |
| ATOM | 333 | ND2 | ASN | 33 | 59.912 | 10.462 | 61.473 | 1.00 | 40.00 |
| ATOM | 336 | C | ASN | 33 | 55.379 | 11.408 | 62.585 | 1.00 | 40.00 |
| ATOM | 337 | O | ASN | 33 | 55.411 | 12.515 | 62.049 | 1.00 | 40.00 |
| ATOM | 338 | N | CYS | 34 | 54.275 | 10.950 | 63.200 | 1.00 | 20.00 |
| ATOM | 340 | CA | CYS | 34 | 53.212 | 11.894 | 63.322 | 1.00 | 20.00 |
| ATOM | 341 | CB | CYS | 34 | 52.404 | 12.098 | 62.032 | 1.00 | 20.00 |
| ATOM | 342 | SG | CYS | 34 | 51.433 | 13.629 | 62.113 | 1.00 | 20.00 |
| ATOM | 343 | C | CYS | 34 | 52.283 | 11.462 | 64.407 | 1.00 | 20.00 |
| ATOM | 344 | O | CYS | 34 | 51.356 | 10.688 | 64.175 | 1.00 | 20.00 |
| ATOM | 345 | N | GLU | 35 | 52.542 | 11.933 | 65.642 | 1.00 | 20.00 |
| ATOM | 347 | CA | GLU | 35 | 51.663 | 11.649 | 66.735 | 1.00 | 20.00 |
| ATOM | 348 | CB | GLU | 35 | 52.196 | 12.161 | 68.084 | 1.00 | 20.00 |
| ATOM | 349 | CG | GLU | 35 | 53.439 | 11.425 | 68.585 | 1.00 | 20.00 |
| ATOM | 350 | CD | GLU | 35 | 53.851 | 12.052 | 69.908 | 1.00 | 20.00 |
| ATOM | 351 | OE1 | GLU | 35 | 54.873 | 11.593 | 70.485 | 1.00 | 20.00 |
| ATOM | 352 | OE2 | GLU | 35 | 53.151 | 12.998 | 70.357 | 1.00 | 20.00 |
| ATOM | 353 | C | GLU | 35 | 50.420 | 12.415 | 66.450 | 1.00 | 20.00 |
| ATOM | 354 | O | GLU | 35 | 49.309 | 11.913 | 66.609 | 1.00 | 20.00 |
| ATOM | 355 | N | VAL | 36 | 50.591 | 13.679 | 66.015 | 1.00 | 20.00 |
| ATOM | 357 | CA | VAL | 36 | 49.445 | 14.482 | 65.726 | 1.00 | 20.00 |
| ATOM | 358 | CB | VAL | 36 | 49.255 | 15.619 | 66.686 | 1.00 | 20.00 |
| ATOM | 359 | CG1 | VAL | 36 | 48.015 | 16.421 | 66.256 | 1.00 | 20.00 |
| ATOM | 360 | CG2 | VAL | 36 | 49.162 | 15.045 | 68.110 | 1.00 | 20.00 |
| ATOM | 361 | C | VAL | 36 | 49.603 | 15.077 | 64.369 | 1.00 | 20.00 |
| ATOM | 362 | O | VAL | 36 | 50.572 | 15.778 | 64.091 | 1.00 | 20.00 |
| ATOM | 363 | N | VAL | 37 | 48.640 | 14.818 | 63.471 | 1.00 | 20.00 |
| ATOM | 365 | CA | VAL | 37 | 48.745 | 15.411 | 62.175 | 1.00 | 20.00 |
| ATOM | 366 | CB | VAL | 37 | 47.997 | 14.656 | 61.101 | 1.00 | 20.00 |
| ATOM | 367 | CG1 | VAL | 37 | 48.665 | 13.282 | 60.929 | 1.00 | 20.00 |
| ATOM | 368 | CG2 | VAL | 37 | 46.508 | 14.540 | 61.476 | 1.00 | 20.00 |
| ATOM | 369 | C | VAL | 37 | 48.173 | 16.787 | 62.307 | 1.00 | 20.00 |
| ATOM | 370 | O | VAL | 37 | 47.002 | 16.964 | 62.634 | 1.00 | 20.00 |
| ATOM | 371 | N | LEU | 38 | 49.011 | 17.816 | 62.095 | 1.00 | 20.00 |
| ATOM | 373 | CA | LEU | 38 | 48.538 | 19.164 | 62.179 | 1.00 | 20.00 |
| ATOM | 374 | CB | LEU | 38 | 49.664 | 20.181 | 62.438 | 1.00 | 20.00 |
| ATOM | 375 | CG | LEU | 38 | 49.181 | 21.640 | 62.533 | 1.00 | 20.00 |
| ATOM | 376 | CD1 | LEU | 38 | 48.220 | 21.843 | 63.715 | 1.00 | 20.00 |
| ATOM | 377 | CD2 | LEU | 38 | 50.372 | 22.614 | 62.561 | 1.00 | 20.00 |
| ATOM | 378 | C | LEU | 38 | 47.938 | 19.486 | 60.856 | 1.00 | 20.00 |
| ATOM | 379 | O | LEU | 38 | 48.632 | 19.915 | 59.936 | 1.00 | 20.00 |
| ATOM | 380 | N | GLY | 39 | 46.610 | 19.300 | 60.738 | 1.00 | 20.00 |
| ATOM | 382 | CA | GLY | 39 | 45.961 | 19.543 | 59.485 | 1.00 | 20.00 |
| ATOM | 383 | C | GLY | 39 | 44.916 | 18.486 | 59.339 | 1.00 | 20.00 |
| ATOM | 384 | O | GLY | 39 | 44.326 | 18.039 | 60.319 | 1.00 | 20.00 |
| ATOM | 385 | N | ASN | 40 | 44.648 | 18.054 | 58.094 | 1.00 | 20.00 |
| ATOM | 387 | CA | ASN | 40 | 43.645 | 17.052 | 57.888 | 1.00 | 20.00 |
| ATOM | 388 | CB | ASN | 40 | 42.481 | 17.526 | 57.002 | 1.00 | 20.00 |
| ATOM | 389 | CG | ASN | 40 | 43.047 | 17.898 | 55.638 | 1.00 | 20.00 |
| ATOM | 390 | OD1 | ASN | 40 | 43.930 | 18.747 | 55.527 | 1.00 | 20.00 |
| ATOM | 391 | ND2 | ASN | 40 | 42.529 | 17.239 | 54.568 | 1.00 | 20.00 |
| ATOM | 394 | C | ASN | 40 | 44.258 | 15.858 | 57.225 | 1.00 | 20.00 |
| ATOM | 395 | O | ASN | 40 | 45.323 | 15.950 | 56.618 | 1.00 | 20.00 |
| ATOM | 396 | N | LEU | 41 | 43.591 | 14.697 | 57.360 | 1.00 | 20.00 |
| ATOM | 398 | CA | LEU | 41 | 44.106 | 13.504 | 56.750 | 1.00 | 20.00 |

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| ATOM | 399 | CB | LEU | 41 | 44.427 | 12.413 | 57.790 | 1.00 | 20.00 |
| ATOM | 400 | CG | LEU | 41 | 44.993 | 11.095 | 57.223 | 1.00 | 20.00 |
| ATOM | 401 | CD1 | LEU | 41 | 43.917 | 10.281 | 56.495 | 1.00 | 20.00 |
| ATOM | 402 | CD2 | LEU | 41 | 46.240 | 11.344 | 56.360 | 1.00 | 20.00 |
| ATOM | 403 | C | LEU | 41 | 43.081 | 13.013 | 55.786 | 1.00 | 20.00 |
| ATOM | 404 | O | LEU | 41 | 41.903 | 12.890 | 56.121 | 1.00 | 20.00 |
| ATOM | 405 | N | GLU | 42 | 43.503 | 12.746 | 54.530 | 1.00 | 20.00 |
| ATOM | 407 | CA | GLU | 42 | 42.576 | 12.236 | 53.573 | 1.00 | 20.00 |
| ATOM | 408 | CB | GLU | 42 | 42.343 | 13.151 | 52.357 | 1.00 | 20.00 |
| ATOM | 409 | CG | GLU | 42 | 41.341 | 12.557 | 51.362 | 1.00 | 20.00 |
| ATOM | 410 | CD | GLU | 42 | 41.171 | 13.525 | 50.199 | 1.00 | 20.00 |
| ATOM | 411 | OE1 | GLU | 42 | 41.827 | 14.601 | 50.222 | 1.00 | 20.00 |
| ATOM | 412 | OE2 | GLU | 42 | 40.384 | 13.201 | 49.271 | 1.00 | 20.00 |
| ATOM | 413 | C | GLU | 42 | 43.131 | 10.961 | 53.033 | 1.00 | 20.00 |
| ATOM | 414 | O | GLU | 42 | 44.302 | 10.892 | 52.659 | 1.00 | 20.00 |
| ATOM | 415 | N | ILE | 43 | 42.304 | 9.899 | 53.011 | 1.00 | 20.00 |
| ATOM | 417 | CA | ILE | 43 | 42.752 | 8.662 | 52.445 | 1.00 | 20.00 |
| ATOM | 418 | CB | ILE | 43 | 42.741 | 7.524 | 53.424 | 1.00 | 20.00 |
| ATOM | 419 | CG2 | ILE | 43 | 43.059 | 6.230 | 52.657 | 1.00 | 20.00 |
| ATOM | 420 | CG1 | ILE | 43 | 43.718 | 7.804 | 54.578 | 1.00 | 20.00 |
| ATOM | 421 | CD1 | ILE | 43 | 45.176 | 7.902 | 54.129 | 1.00 | 20.00 |
| ATOM | 422 | C | ILE | 43 | 41.784 | 8.327 | 51.358 | 1.00 | 20.00 |
| ATOM | 423 | O | ILE | 43 | 40.727 | 7.756 | 51.616 | 1.00 | 20.00 |
| ATOM | 424 | N | THR | 44 | 42.126 | 8.643 | 50.096 | 1.00 | 20.00 |
| ATOM | 426 | CA | THR | 44 | 41.172 | 8.389 | 49.058 | 1.00 | 20.00 |
| ATOM | 427 | CB | THR | 44 | 40.818 | 9.607 | 48.256 | 1.00 | 20.00 |
| ATOM | 428 | OG1 | THR | 44 | 39.737 | 9.316 | 47.382 | 1.00 | 20.00 |
| ATOM | 430 | CG2 | THR | 44 | 42.053 | 10.050 | 47.453 | 1.00 | 20.00 |
| ATOM | 431 | C | THR | 44 | 41.667 | 7.354 | 48.098 | 1.00 | 20.00 |
| ATOM | 432 | O | THR | 44 | 42.868 | 7.121 | 47.968 | 1.00 | 20.00 |
| ATOM | 433 | N | TYR | 45 | 40.704 | 6.690 | 47.429 | 1.00 | 20.00 |
| ATOM | 435 | CA | TYR | 45 | 40.919 | 5.707 | 46.405 | 1.00 | 20.00 |
| ATOM | 436 | CB | TYR | 45 | 41.028 | 6.314 | 44.994 | 1.00 | 20.00 |
| ATOM | 437 | CG | TYR | 45 | 39.706 | 6.904 | 44.639 | 1.00 | 20.00 |
| ATOM | 438 | CD1 | TYR | 45 | 38.687 | 6.101 | 44.182 | 1.00 | 20.00 |
| ATOM | 439 | CE1 | TYR | 45 | 37.480 | 6.645 | 43.808 | 1.00 | 20.00 |
| ATOM | 440 | CD2 | TYR | 45 | 39.503 | 8.263 | 44.708 | 1.00 | 20.00 |
| ATOM | 441 | CE2 | TYR | 45 | 38.298 | 8.812 | 44.337 | 1.00 | 20.00 |
| ATOM | 442 | CZ | TYR | 45 | 37.284 | 8.002 | 43.884 | 1.00 | 20.00 |
| ATOM | 443 | OH | TYR | 45 | 36.051 | 8.560 | 43.489 | 1.00 | 20.00 |
| ATOM | 445 | C | TYR | 45 | 42.127 | 4.854 | 46.623 | 1.00 | 20.00 |
| ATOM | 446 | O | TYR | 45 | 43.049 | 4.867 | 45.811 | 1.00 | 20.00 |
| ATOM | 447 | N | VAL | 46 | 42.169 | 4.080 | 47.723 | 1.00 | 20.00 |
| ATOM | 449 | CA | VAL | 46 | 43.301 | 3.215 | 47.895 | 1.00 | 20.00 |
| ATOM | 450 | CB | VAL | 46 | 44.235 | 3.641 | 48.988 | 1.00 | 20.00 |
| ATOM | 451 | CG1 | VAL | 46 | 43.474 | 3.627 | 50.320 | 1.00 | 20.00 |
| ATOM | 452 | CG2 | VAL | 46 | 45.461 | 2.713 | 48.965 | 1.00 | 20.00 |
| ATOM | 453 | C | VAL | 46 | 42.811 | 1.841 | 48.220 | 1.00 | 20.00 |
| ATOM | 454 | O | VAL | 46 | 41.745 | 1.678 | 48.813 | 1.00 | 20.00 |
| ATOM | 455 | N | GLN | 47 | 43.573 | 0.802 | 47.815 | 1.00 | 20.00 |
| ATOM | 457 | CA | GLN | 47 | 43.130 | -0.533 | 48.099 | 1.00 | 20.00 |
| ATOM | 458 | CB | GLN | 47 | 42.333 | -1.150 | 46.940 | 1.00 | 20.00 |
| ATOM | 459 | CG | GLN | 47 | 41.063 | -0.367 | 46.607 | 1.00 | 20.00 |
| ATOM | 460 | CD | GLN | 47 | 40.429 | -1.005 | 45.381 | 1.00 | 20.00 |
| ATOM | 461 | OE1 | GLN | 47 | 39.658 | -1.958 | 45.483 | 1.00 | 20.00 |
| ATOM | 462 | NE2 | GLN | 47 | 40.771 | -0.468 | 44.180 | 1.00 | 20.00 |
| ATOM | 465 | C | GLN | 47 | 44.309 | -1.426 | 48.332 | 1.00 | 20.00 |
| ATOM | 466 | O | GLN | 47 | 45.210 | -1.490 | 47.501 | 1.00 | 20.00 |
| ATOM | 467 | N | ARG | 48 | 44.353 | -2.119 | 49.490 | 1.00 | 20.00 |
| ATOM | 469 | CA | ARG | 48 | 45.386 | -3.099 | 49.670 | 1.00 | 20.00 |
| ATOM | 470 | CB | ARG | 48 | 46.828 | -2.580 | 49.817 | 1.00 | 20.00 |
| ATOM | 471 | CG | ARG | 48 | 47.112 | -1.831 | 51.115 | 1.00 | 20.00 |
| ATOM | 472 | CD | ARG | 48 | 48.611 | -1.746 | 51.417 | 1.00 | 20.00 |
| ATOM | 473 | NE | ARG | 48 | 49.145 | -3.137 | 51.474 | 1.00 | 20.00 |

| | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|
| ATOM | 475 | CZ | ARG | 48 | 50.483 | -3.358 | 51.318 | 1.00 | 20.00 |
| ATOM | 476 | NH1 | ARG | 48 | 50.973 | -4.631 | 51.348 | 1.00 | 20.00 |
| ATOM | 479 | NH2 | ARG | 48 | 51.331 | -2.307 | 51.125 | 1.00 | 20.00 |
| ATOM | 482 | C | ARG | 48 | 45.108 | -3.855 | 50.928 | 1.00 | 20.00 |
| ATOM | 483 | O | ARG | 48 | 44.103 | -3.633 | 51.600 | 1.00 | 20.00 |
| ATOM | 484 | N | ASN | 49 | 46.020 | -4.783 | 51.272 | 1.00 | 20.00 |
| ATOM | 486 | CA | ASN | 49 | 45.864 | -5.613 | 52.430 | 1.00 | 20.00 |
| ATOM | 487 | CB | ASN | 49 | 46.987 | -6.657 | 52.557 | 1.00 | 20.00 |
| ATOM | 488 | CG | ASN | 49 | 46.858 | -7.627 | 51.393 | 1.00 | 20.00 |
| ATOM | 489 | OD1 | ASN | 49 | 45.806 | -8.228 | 51.183 | 1.00 | 20.00 |
| ATOM | 490 | ND2 | ASN | 49 | 47.957 | -7.781 | 50.607 | 1.00 | 20.00 |
| ATOM | 493 | C | ASN | 49 | 45.891 | -4.796 | 53.682 | 1.00 | 20.00 |
| ATOM | 494 | O | ASN | 49 | 44.996 | -4.901 | 54.518 | 1.00 | 20.00 |
| ATOM | 495 | N | TYR | 50 | 46.917 | -3.937 | 53.835 | 1.00 | 20.00 |
| ATOM | 497 | CA | TYR | 50 | 47.034 | -3.184 | 55.049 | 1.00 | 20.00 |
| ATOM | 498 | CB | TYR | 50 | 48.313 | -2.332 | 55.148 | 1.00 | 20.00 |
| ATOM | 499 | CG | TYR | 50 | 49.476 | -3.249 | 55.318 | 1.00 | 20.00 |
| ATOM | 500 | CD1 | TYR | 50 | 49.774 | -3.761 | 56.559 | 1.00 | 20.00 |
| ATOM | 501 | CE1 | TYR | 50 | 50.869 | -4.574 | 56.740 | 1.00 | 20.00 |
| ATOM | 502 | CD2 | TYR | 50 | 50.301 | -3.547 | 54.258 | 1.00 | 20.00 |
| ATOM | 503 | CE2 | TYR | 50 | 51.398 | -4.359 | 54.433 | 1.00 | 20.00 |
| ATOM | 504 | CZ | TYR | 50 | 51.683 | -4.873 | 55.675 | 1.00 | 20.00 |
| ATOM | 505 | OH | TYR | 50 | 52.810 | -5.702 | 55.857 | 1.00 | 20.00 |
| ATOM | 507 | C | TYR | 50 | 45.871 | -2.269 | 55.220 | 1.00 | 20.00 |
| ATOM | 508 | O | TYR | 50 | 45.151 | -1.960 | 54.272 | 1.00 | 20.00 |
| ATOM | 509 | N | ASP | 51 | 45.658 | -1.829 | 56.476 | 1.00 | 40.00 |
| ATOM | 511 | CA | ASP | 51 | 44.594 | -0.929 | 56.799 | 1.00 | 40.00 |
| ATOM | 512 | CB | ASP | 51 | 43.591 | -1.486 | 57.825 | 1.00 | 40.00 |
| ATOM | 513 | CG | ASP | 51 | 42.761 | -2.572 | 57.151 | 1.00 | 40.00 |
| ATOM | 514 | OD1 | ASP | 51 | 42.891 | -2.734 | 55.908 | 1.00 | 40.00 |
| ATOM | 515 | OD2 | ASP | 51 | 41.978 | -3.250 | 57.869 | 1.00 | 40.00 |
| ATOM | 516 | C | ASP | 51 | 45.238 | 0.271 | 57.414 | 1.00 | 40.00 |
| ATOM | 517 | O | ASP | 51 | 46.447 | 0.299 | 57.629 | 1.00 | 40.00 |
| ATOM | 518 | N | LEU | 52 | 44.426 | 1.306 | 57.692 | 1.00 | 40.00 |
| ATOM | 520 | CA | LEU | 52 | 44.875 | 2.544 | 58.259 | 1.00 | 40.00 |
| ATOM | 521 | CB | LEU | 52 | 43.795 | 3.638 | 58.253 | 1.00 | 40.00 |
| ATOM | 522 | CG | LEU | 52 | 44.316 | 5.001 | 58.745 | 1.00 | 40.00 |
| ATOM | 523 | CD1 | LEU | 52 | 45.417 | 5.540 | 57.819 | 1.00 | 40.00 |
| ATOM | 524 | CD2 | LEU | 52 | 43.167 | 6.001 | 58.947 | 1.00 | 40.00 |
| ATOM | 525 | C | LEU | 52 | 45.316 | 2.310 | 59.672 | 1.00 | 40.00 |
| ATOM | 526 | O | LEU | 52 | 46.083 | 3.086 | 60.238 | 1.00 | 40.00 |
| ATOM | 527 | N | SER | 53 | 44.838 | 1.207 | 60.272 | 1.00 | 40.00 |
| ATOM | 529 | CA | SER | 53 | 45.077 | 0.879 | 61.649 | 1.00 | 40.00 |
| ATOM | 530 | CB | SER | 53 | 44.492 | -0.484 | 62.049 | 1.00 | 40.00 |
| ATOM | 531 | OG | SER | 53 | 45.162 | -1.527 | 61.355 | 1.00 | 40.00 |
| ATOM | 533 | C | SER | 53 | 46.536 | 0.824 | 61.965 | 1.00 | 40.00 |
| ATOM | 534 | O | SER | 53 | 46.923 | 1.047 | 63.111 | 1.00 | 40.00 |
| ATOM | 535 | N | PHE | 54 | 47.391 | 0.535 | 60.967 | 1.00 | 40.00 |
| ATOM | 537 | CA | PHE | 54 | 48.788 | 0.373 | 61.250 | 1.00 | 40.00 |
| ATOM | 538 | CB | PHE | 54 | 49.665 | 0.050 | 60.021 | 1.00 | 40.00 |
| ATOM | 539 | CG | PHE | 54 | 49.742 | 1.221 | 59.103 | 1.00 | 40.00 |
| ATOM | 540 | CD1 | PHE | 54 | 50.664 | 2.219 | 59.322 | 1.00 | 40.00 |
| ATOM | 541 | CD2 | PHE | 54 | 48.995 | 1.254 | 57.950 | 1.00 | 40.00 |
| ATOM | 542 | CE1 | PHE | 54 | 50.813 | 3.247 | 58.419 | 1.00 | 40.00 |
| ATOM | 543 | CE2 | PHE | 54 | 49.127 | 2.284 | 57.049 | 1.00 | 40.00 |
| ATOM | 544 | CZ | PHE | 54 | 50.040 | 3.284 | 57.283 | 1.00 | 40.00 |
| ATOM | 545 | C | PHE | 54 | 49.319 | 1.607 | 61.908 | 1.00 | 40.00 |
| ATOM | 546 | O | PHE | 54 | 50.271 | 1.519 | 62.680 | 1.00 | 40.00 |
| ATOM | 547 | N | LEU | 55 | 48.738 | 2.790 | 61.609 | 1.00 | 40.00 |
| ATOM | 549 | CA | LEU | 55 | 49.180 | 4.002 | 62.248 | 1.00 | 40.00 |
| ATOM | 550 | CB | LEU | 55 | 48.495 | 5.271 | 61.707 | 1.00 | 40.00 |
| ATOM | 551 | CG | LEU | 55 | 48.790 | 5.573 | 60.228 | 1.00 | 40.00 |
| ATOM | 552 | CD1 | LEU | 55 | 50.281 | 5.855 | 60.008 | 1.00 | 40.00 |
| ATOM | 553 | CD2 | LEU | 55 | 48.248 | 4.478 | 59.299 | 1.00 | 40.00 |

Annexure A

AUSTRALIA

Patents Act 1990

COMMONWEALTH SCIENTIFIC AND INDUSTRIAL RESEARCH ORGANISATION

PROVISIONAL SPECIFICATION

Invention Title:

EGF family receptor agonists and antagonists

The invention is described in the following statement:

EGF FAMILY RECEPTOR AGONISTS AND ANTAGONISTS

Field of the Invention

This invention relates to the field of receptor structure and receptor/ligand interactions. In particular it relates to the field of using
5 receptor structure to predict the structure of related receptors and to use the determined structures and predicted structures to select and screen for agonists and antagonists of the polypeptide ligands.

Background of the Invention

Insulin is the peptide hormone that regulates glucose uptake and
10 metabolism. The two types of diabetes are associated with either an inability to produce insulin because of destruction of the pancreatic islet cells (Homo-Delarche, F. & Boitard, C., 1996, Immunol. Today 10: 456-460) or poor glucose metabolism resulting from either insulin resistance at the target tissues, inadequate insulin secretion by the islets or faulty liver function (Taylor, S.
15 I., et al., 1994, Diabetes, 43: 735-740).

Insulin-like growth factors-1 and 2 (IGF-1 and 2) are structurally related to insulin but are more important in tissue growth and development than in metabolism. They are primarily produced in the liver in response to growth hormone but are also produced in most other tissues where they
20 function as paracrine/autocrine regulators. The IGFs are strong mitogens and are involved in numerous physiological states and certain cancers (Baserga, R., 1996, TibTech 14: 150-152).

Epidermal growth factor (EGF) is a small polypeptide cytokine that is unrelated to the insulin/IGF family. It stimulates marked proliferation of
25 epithelial tissues and is a member of a larger family of structurally related cytokines such as transforming growth factor α , amphiregulin, betacellulin, heparin-binding EGF and some viral gene products. Abnormal EGF family signalling is a characteristic of certain cancers (Soler, C. & Carpenter, G., 1994 In Nicola, N. (ed) Guidebook to Cytokines and Their receptors", Oxford Univ. Press, Oxford, pp194-197; Walker, F. & Burgess, A. W., 1994, In Nicola, N. (ed) Guidebook to Cytokines and Their receptors", Oxford Univ. Press,
30 Oxford, pp198-201).

Each of these growth factors mediate their biological actions through binding to the corresponding receptor. The IR, IGF-1R and insulin receptor-related receptor (IRR), for which the ligand is not known, are closely related
35 to each other and are referred to as the insulin receptor subfamily. There is a

large body of information now available concerning the primary structure of these insulin receptor subfamily members (Ebina, Y., et al., 1985 *Cell* 40: 747-758; Ullrich, A., et al., 1985, *Nature* 313: 756-761; Ullrich, A. et al., 1986, *EMBO J* 5: 2503-2512; Shier, P. & Watt, V. M., 1989, *J. Biol. Chem.* 264: 14605-14608) and the identification of some of their functional domains (for reviews see De Meyts, P. 1994, *Diabetologia* 37: 135-148; Lee, J. & Pilch, P. F. 1994 *Amer. J. Physiol.* 266: C319-C334.; Schaffer, L. 1994, *Eur. J. Biochem.* 221: 1127-1132). IGF-1R, IR and IRR are members of the tyrosine kinase receptor superfamily and are closely related to the epidermal growth factor receptor (EGFR) subfamily, with which they share significant sequence identity in the extracellular region as well as in the cytoplasmic kinase domains (Ullrich, A. et al., 1984 *Nature* 309: 418-425; Ward, C. W. et al., 1995 *Proteins: Structure Function & Genetics* 22: 141-153). Both the insulin and EGF receptor subfamilies have a similar arrangement of two homologous domains (L1 and L2) separated by a cys-rich region of approximately 160 amino acids containing 22-24 cys residues (Bajaj, M., et al., 1987 *Biochim. Biophys. Acta* 916: 220-226; Ward, C. W. et al., 1995 *Proteins: Structure Function & Genetics* 22: 141-153). The C-terminal portion of the IGF-1R ectodomain (residues 463 to 906) is comprised of four domains: a connecting domain, two fibronectin type 3 (Fn3) repeats, and an insert domain (O'Bryan, J. P., et al., 1991 *Mol Cell Biol* 11: 5016-5031); the C-terminal portion of the EGFR ectodomain (residues 477-621) consists solely of a second cys-rich region containing 20 cys residues (Ullrich, A. et al., 1984, *Nature* 309: 418-425).

Little is known about the secondary, tertiary and quaternary structure of the ectodomains of these receptor subfamilies. Unlike the members of the EGFR subfamily which are transmembrane monomers which dimerise on binding ligand, the IR subfamily members are homodimers, held together by disulphide bonds. The extracellular region of the IR/IGF-1R/IRR monomers contains an α -chain (~ 703 to 735 amino acid residues) and 192-196 residues of the β -chain. There is a ~23 residue transmembrane segment, followed by the cytoplasmic portion (354 to 408 amino acids) which contains the catalytic tyrosine kinase domain flanked by juxtamembrane and C-tail regulatory regions and is responsible for mediating all receptor-specific functions (White, M. F. & Kahn, C. R. 1994 *J. Biol. Chem.* 269: 1-4). Chemical analyses of the receptor suggest that the α -chains are linked to the β -chains

via a single disulphide bond with the IR dimer being formed by at least two α - α disulphide linkages (Finn, F. M., et al., 1990, *Proc. Natl. Acad. Sci.* 87: 419-423; Chiacchia, K. B., 1991, *Biochem. Biophys. Res. Commun.* 176, 1178-1182; Schaffer, L. & Ljungqvist, L., 1992, *Biochem. Biophys. Res. Commun.* 189: 650-653; Sparrow, L. G., et al., 1997, *J. Biol. Chem.* 272: 29460-29467).

Although the 3D structures of the ligands EGF, TGF- α (Hommel, U., et al., 1992, *J. Mol. Biol.* 227:271-282), insulin (Dodson, E. J., et al., 1983, *Biopolymers* 22:281-291), IGF-1 (Sato, A., et al., 1993, *Int J Peptide Protein Res* 41:433-440) and IGF-2 (Torres, A. M., et al., 1995, *J. Mol. Biol.* 248:385-401) are known and numerous analytical and functional studies of ligand binding to EGFR (Soler, C. & Carpenter, G., 1994 In Nicola (ed) *Guidebook to Cytokines and Their receptors*, Oxford Univ. Press, Oxford, pp194-197), IGF-1R and IR (see De Meyts, P., 1994 *Diabetologia*, 37:135-148) have been carried out, the mechanisms of ligand binding and subsequent transmembrane signalling have not been resolved.

Ligand-induced, receptor-mediated phosphorylation is the signalling mechanism by which most cytokines, polypeptide hormones and membrane-anchored ligands exert their biological effects. The primary kinase may be part of the intracellular portion of the transmembrane receptor protein as in the tyrosine kinase receptors (for review see Yarden, Y., et al., 1988, *Ann. Rev. Biochem.* 57:443-478) or the Ser/Thr kinase receptors (Alevizopoulos, A. & Mermoud, N., 1997, *BioEssays*, 19:581-591) or be non-covalently associated with the cytoplasmic tail of the transmembrane protein(s) making up the receptor complex as in the case of the haemopoietic growth factor receptors (Stahl, N., et al., 1995, *Science* 267:1349-1353). The end result is the same, ligand binding leads to receptor dimerization or oligomerization or a conformational change in pre-existing receptor dimers or oligomers resulting in activation by transphosphorylation, of the covalently attached or non-covalently associated protein kinase domains (Hunter, T., 1995, *Cell*, 80:225-236).

Many oncogenes have been shown to be homologous to growth factors, growth factor receptors or molecules in the signal transduction pathways (Baserga, R., 1994 *Cell*, 79:927-930; Hunter, T., 1997 *Cell*, 88:333-346). One of the best examples is v-Erb (related to the EGFR). Since overexpression of a number of growth factor receptors results in ligand-dependent transformation an alternate strategy for oncogenes is to regulate

the expression of growth factor receptors or their ligands or to directly bind to the receptors to stimulate the same effect (Baserga, R., 1994 Cell, 79:927-930). Examples are v-Src, which activates IGF-1 R intracellularly; c-Myb, which transforms cells by enhancing the expression of IGF1R and SV40 T antigen which interacts with the IGF-1R and enhances the secretion of IGF-1 (see Baserga, R., 1994 Cell, 79:927-930 for review). Cells in which the IGF-1 receptor has been knocked out cannot be transformed by SV40 T antigen. If oncogenes activate growth factors and their receptors then tumour suppressor genes should have the opposite effect. One good example of this is WT1, the Wilm's tumour suppressor gene which suppresses the expression of IGF-1R (Drummond, J. A., et al., 1992, Science, 257:275-277). Cells that are driven to proliferate by oncogenes undergo massive apoptosis when growth factor receptors are ablated since unlike normal cells, they appear unable to withdraw from the cell-cycle and enter into the G0 phase (Baserga, R., 1994 Cell, 79:927-930).

The insulin-like growth factor-1 receptor (IGF-1R) is one of several growth-factor receptors that regulate the proliferation of mammalian cells. However, its ubiquitousness and certain unique aspects of its function make IGF-1R an ideal target for therapeutic interventions against abnormal growth, with very little effect on normal cells (see Baserga, R., 1996 TIBTECH, 14:150-152). The receptor is activated by IGF1, IGF2 and insulin and plays a major role in cellular proliferation in at least three ways: it is essential for optimal growth of cells in vitro and in vivo; several cell types require IGF-1R to maintain the transformed state and activated IGF-1R has a protective effect against apoptotic cell death (Baserga, R., 1996 TIBTECH, 14:150-152). These properties alone make it an ideal target for therapeutic interventions. Transgenic experiments have shown that IGF-1R is not an absolute requirement for cell growth but is essential for the establishment of the transformed state (Baserga, R., 1994 Cell, 79: 927-930). In several cases (human glioblastoma, human melanoma; human breast carcinoma; human lung carcinoma; human ovarian carcinoma; human rhabdomyosarcoma; mouse melanoma, mouse leukaemia; rat glioblastoma; rat rhabdomyosarcoma; hamster mesothelioma) the transformed phenotype can be reversed by decreasing the expression of IGF-1R using antisense to IGF-1R (Baserga, R., 1996 TIBTECH 14:150-152); or interfering with its function by antibodies to IGF-1R (human breast carcinoma; human rhabdomyosarcoma)

or by dominant negatives of IGF-1R (rat glioblastoma; Baserga, R., 1996 TIBTECH 14:150-152).

Three effects are observed when the function of IGF-1R is impaired: tumour cells undergo massive apoptosis which results in inhibition of tumourogenesis; surviving tumour cells are eliminated by a specific immune response; and such a host response can cause a regression of an established wild-type tumour (Resnicoff, M., et al., 1995, Cancer Res. 54:2218-2222). These effects, plus the fact that interference of IGF-1R function has a limited effect on normal cells (partial inhibition of growth without apoptosis) makes IGF-1R a unique target for therapeutic interventions (Baserga, R., 1996 TIBTECH 14:150-152). In addition IGF-1R is downstream of many other growth factor receptors, which makes it an even more generalised target. The implication of these findings is that if you can decrease the number of IGF-1 receptors on cells or antagonise their function then tumours cease to grow and can be removed immunologically. These studies establish that IGF-1R antagonists will be extremely important therapeutically.

Many cancer cells have constitutively active EGFR (Sandgreen, E. P., et al., 1990, Cell, 61:1121-135; Karnes, W. E. J., et al., 1992, Gastroenterology, 102:474-485) or other EGFR family members (Hines, N. E., 1993, Semin. Cancer Biol. 4:19-26). Elevated levels of activated EGFR occur in bladder, breast, lung and brain tumours (Harris, A. L., et al., 1989, In Furth & Greaves (eds) The Molecular Diagnostics of human cancer. Cold Spring Harbor Lab. Press, CSH, NY, pp353-357). Antibodies to EGFR can inhibit ligand activation of EGFR (Sato, J. D., et al., 1983 Mol. Biol. Med. 1:511-529) and the growth of many epithelial cell lines (Aboud-Pirak E., et al., 1988, J. Natl Cancer Inst. 85:1327-1331). Patients receiving repeated doses of a humanised chimeric anti-EGFR antibody showed signs of disease stabilization. The large doses required and the cost of production of humanised Mab is likely to limit the application of this type of therapy. These findings indicate that the development of EGF antagonists will be attractive anticancer agents.

Summary of the Invention

The present inventors have now obtained 3D structural information concerning the insulin-like growth factor receptor (IGF-1R) and the insulin receptor (IR) which provides a rational basis for the development of antagonists and agonists of the polypeptide ligands for specific therapeutic applications. This information can be used to predict the structure of related

members of the insulin receptor family and epidermal growth factor family and to develop agonists and antagonists of their respective polypeptide ligands.

Accordingly, in a first aspect the present invention provides a method of screening for, or designing, an agonist of a ligand of an insulin receptor family member or EGF receptor family member which method includes

(i) selecting or designing a substance which possesses stereochemical complementarity to a receptor site, wherein the receptor site is characterised by

(a) amino acids 1-462 of IGF-1R positioned at atomic coordinates substantially as shown in Figure 1 or a subset thereof; or

(b) amino acids derived from an insulin receptor family member or EGF receptor family member which form an equivalent structure to the amino acids defined in paragraph (a); and

(ii) testing the substance for the ability to act as an agonist of the ligand of an insulin receptor family member or EGF receptor family member.

In a second aspect the present invention provides a method of screening for, or designing, an antagonist of a ligand of an insulin receptor family member or EGF receptor family member which method includes

(i) selecting or designing a substance which possesses stereochemical complementarity to a receptor site, wherein the receptor site is characterised by

(a) amino acids 1-462 of IGF-1R positioned at atomic coordinates substantially as shown in Figure 1 or a subset thereof; or

(b) amino acids derived from an insulin receptor family member or an EGF receptor family member which form an equivalent structure to the amino acids defined in paragraph (a); and

(ii) testing the substance for the ability to act as an antagonist of the ligand of an insulin receptor family member or EGF receptor family member.

The phrase "insulin receptor family" encompasses, for example, IGF-1R, IR and IRR. The phrase "EGF receptor family" encompasses for example, EGFR, ErbB2, ErbB3 and ErbB4. In general, insulin receptor family members and EGF receptor family members show similar domain arrangements and share significant sequence identity (preferably at least 20% identity between the families and at least 40% identity within each family).

The receptor site defined in the first and second aspects of the present invention comprises the L1-cysteine rich-L2 region (residues 1-462) of the ectodomain of IGF-1R. At the centre of this structure is a groove, bounded by all three domains, of sufficient size to accommodate a ligand molecule. By "stereochemical complementarity" we mean that the biologically active substance or a portion thereof correlates, in the manner of the classic "lock-and-key" visualisation of ligand-receptor interaction, with the groove in the receptor site. Preferably, the stereochemical complementarity is such that the compound has a K_i for the receptor site of less than $10^{-6}M$. More preferably, the K_i value is less than $10^{-8}M$ and more preferably less than $10^{-9}M$.

In preferred embodiments of the first and second aspects of the present invention, the method further involves selecting or designing a substance which has portions that match residues positioned on the surface of the receptor site which faces the groove. By "match" we mean that the identified portions interact with the surface residues, for example, via hydrogen bonding or by enthalpy-reducing Van der Waals interactions which promote desolvation of the biologically active substance within the site, in such a way that retention of the biologically active substance within the groove is favoured energetically.

In a preferred embodiment of the first aspect of the present invention, the method includes screening for, or designing, a substance which possesses a stereochemistry and/or geometry which allows it to interact with both the L1 and L2 domains of the receptor site. As described above, the insulin receptor exists as homodimers held together by disulphide bonds. Electron microscopy studies described herein indicate that the insulin receptor monomers dimerise in nature in such a manner that the grooves of each monomer may face each other. Accordingly, the method of the first aspect of the present invention may involve screening for, or designing, a biologically active substance which interacts with the L1 domain of one monomer and the L2 domain of the other monomer.

In a third aspect the present invention provides a method of selecting or designing an agonist of a ligand of an insulin receptor family member or EGF receptor family member which method includes

(i) selecting or designing a substance which interacts with

(a) a fragment of IGF-1R characterised by amino acids 1-462 positioned at atomic coordinates substantially as shown in Figure 1 or a subset thereof; or

5 (b) a fragment derived from an insulin family receptor member or EGF receptor family member which is equivalent to the fragment defined in paragraph (a);

wherein the interaction of the substance with the fragment alters the position of at least one of the L1, L2 or cys-rich domains of the fragment relative to the position of at least one of the other domains; and

10 (ii) testing the substance for the ability to act as an agonist of the ligand of an insulin receptor family member or EGF receptor family member.

In a preferred embodiment of the third aspect of the present invention the substance interacts with the fragment in the region of the L1 domain-cys rich domain interface, causing the L1 and cys-rich domains to
15 move away from each other. In a further preferred embodiment the substance interacts with the hinge region between the L2 domain and the cys-rich domain causing an alteration in the positions of the domains relative to each other. In a further preferred embodiment the substance interacts with the beta sheet of the L1 domain causing an alteration in the position of
20 the L1 domain relative to the position of the cys-rich domain or L2 domain.

In a fourth aspect the present invention provides an agonist of a ligand of an insulin receptor family member or EGF receptor family member obtained by a method according to the first or third aspects of the present invention.

25 In a fifth aspect the present invention provides an antagonist of ligand of an insulin receptor family member or EGF receptor family member obtained by a method according to the second aspect of the present invention.

The agonists or antagonists of the fourth and fifth aspects of the
30 present invention may be mutant insulin family member or EGF family member ligands where at least one mutation occurs in the region of the ligand which interacts with residues on the surface of the receptor site facing toward the groove. For example, the IGF-1 ligand has a predominance of basic residues in the C region which may interact with the acidic patch of the
35 cys-rich region near L1. An acidic patch on the other side of the ligand may interact with the patch of basic residues (residues 307-310) on the N-terminal

end of L2. Accordingly, mutants of IGF-1 which exhibit altered activity may be generated by introducing modifications in the C region of IGF-1 or residues in the acidic patch on the other side of the hormone.

5 In a sixth aspect the present invention provides a substance which possesses stereochemical complementarity to a receptor site, wherein the receptor site is characterised by

(a) amino acids 1-462 of IGF-1R positioned at atomic coordinates substantially as shown in Figure 1 or a subset thereof; or

10 (b) amino acids derived from an insulin receptor family member or an EGF receptor family member which form an equivalent structure to the amino acids defined in paragraph (a);

with the proviso that the substance is not a naturally occurring ligand of an insulin receptor family member or EGF receptor family member or a mutant thereof.

15 By "mutant" we mean a ligand which has been modified by one or more point mutations, insertions of amino acids or deletions of amino acids.

In a preferred embodiment of the sixth aspect of the present invention, the stereochemical complementarity is such that the compound has a K_i for the receptor site of less than $10^{-6}M$. More preferably, the K_i value
20 is less than $10^{-8}M$ and more preferably less than $10^{-9}M$.

In a seventh aspect the present invention provides a pharmaceutical composition for treatment of a disease associated with reduced activity of a ligand of an insulin receptor family member or EGF receptor family member which includes an agonist obtained by a method according to the first or
25 third aspects of the present invention and a pharmaceutically acceptable carrier or diluent.

In an eighth aspect the present invention provides a pharmaceutical composition for treatment of a disease associated with activity of a ligand of an insulin receptor family member or EGF receptor family member which
30 includes an antagonist obtained by a method according to the second aspect of the present invention and a pharmaceutically acceptable carrier or diluent.

In a ninth aspect the present invention provides a method of preventing or treating a disease associated with reduced activity of a ligand of an insulin receptor family member or EGF receptor family member which
35 method includes administering to a subject in need thereof an agonist

obtained by a method according to the first or third aspects of the present invention.

Diseases associated with reduced activity of a ligand of an insulin receptor family member or EGF receptor family member include diabetes, osteoporosis, nerve degeneration and a range of catabolic states.

In a tenth aspect the present invention provides a method of preventing or treating a disease associated with activity of a ligand of an insulin receptor family member or EGF receptor family member which method includes administering to a subject in need thereof an antagonist obtained by a method according to the second aspect of the present invention.

Diseases associated with activity of a ligand of an insulin receptor family member or EGF receptor family member include cancer, leukaemia and many types of tumour states including but not restricted to breast cancer, brain tumours, ovarian cancer, pancreatic tumours, lung cancer, melanoma, rhabdomyosarcoma, mesothelioma and glioblastoma.

Brief Description of the Drawings

Figure 1. IGF-1R residues 1-462, in terms of atomic coordinates refined to a resolution of 2.6 Å (average accuracy \approx 0.3Å). The coordinates are in relation to a Cartesian system of orthogonal axes.

Figure 2. Depiction of the residues lining the groove of the IGF-1R receptor fragment 1-462.

Figure 3. Gel filtration chromatography of affinity-purified IGF-1R/462 protein. The protein was purified on a Superdex S200 column (Pharmacia) fitted to a BioLogic L.C. system (Biorad), equilibrated and eluted at 0.8 ml/min with 40 mM Tris/150 mM NaCl/0.02% NaN₃ adjusted to pH 8.0. (a) Protein eluting in peak 1 contained aggregated IGF-1R/462 protein, peak 2 contained monomeric protein and peak 3 contained the c-myc undecapeptide used for elution from the Mab 9E10 immunoaffinity column. (b) Non-reduced SDS-PAGE of fraction 2 from IGF-1R/462 obtained following Superdex S200 (Fig.1a). Standard proteins are indicated.

Figure 4. Ion exchange chromatography of affinity-purified, truncated IGF-1R ectodomain. A mixture of gradient and isocratic elution chromatography was performed on a Resource Q column (Pharmacia) fitted to a BioLogic System (Biorad), using 20 mM Tris/pH 8.0 as buffer A and the same buffer containing 1M NaCl as buffer B. Protein solution in TBSA was diluted at least 1:2 with water and loaded onto the column at 2 ml/min. Elution was monitored by absorbance (280 nm) and conductivity (mS/cm). Target protein (peak 2) eluted isocratically with 20 mM Tris/0.14 M NaCl pH 8.0. Inset: Isoelectric focusing gel (pH 3 - 7; Novex Australia Pty Ltd) of fraction 2. The pI was estimated at 5.1 from standard proteins (not shown).

Figure 5. Gel filtration chromatography of affinity purified IR/485 protein. Affinity-purified material at 1 mg/ml produced a dominant peak at apparent mass ~ 140 kDa (interpreted as a dimer) (a); whereas affinity-purified material at 0.02 mg/ml produced a dominant peak at apparent mass ~ 85kDa (interpreted as a monomer) (b).

Figure 6. (a) SDS-PAGE of IR/485 following gel filtration chromatography. The protein migrated as a single broad band of apparent molecular mass ~ 78 kDa (reduced - lane A) or ~ 68kDa (non-reduced - lane B). (b) Isoelectric focussing of the IR/485 protein. The IR/485 fragment reacted positively in an ELISA with Mab 83-7, gave a single sequence corresponding to the N-terminal 10 residues of IR, showing several isoforms on isoelectric focussing from pI6.0-6.8. The fragment was further purified by ion-exchange chromatography on Uno Q (BioRad, USA), using stepwise isocratic elution with incremental changes in salt concentrations (see Figure 7). Fractions A and D were each enriched in a component isoform from the ladder of isoforms present in the unfractionated mixture. Both these fractions produced crystals, whereas no crystals were obtained from fractions B and C.

Figure 7. Purification of the IR/485 protein by ion-exchange chromatography on Uno Q (BioRad, USA), using stepwise isocratic elution with incremental changes in salt concentrations.

Figure 8. Polypeptide fold for residues 1-462 of IGF-1R. The L1 domain is at the top, viewed from the N-terminal end and L2 is at the bottom. The space

at the centre is of sufficient size to accommodate IGF-1. Helices are indicated by curled ribbon and β -strands by arrows. Cysteine side chains are drawn as ball-and-stick with lines showing disulfide bonds. The arrow points in the direction of view for Figure 9.

5

Figure 9. Amino acid sequences of IGF-1R and related proteins. a, L1 and L2 domains of human IGF-1R and IR are shown based on a sequence alignment for the two proteins and a structural alignment for the L1 and L2 domains. Positions showing conservation physico-chemical properties of amino acids are boxed, residues used in the structural alignment are shaded yellow and residues which form the Trp 176 pocket are in red. Secondary structure elements for L1 (above the sequences) and L2 (below) are indicated as cylinders for helices and arrows for β -strands. Strands are colour coded according to the β -sheet to which they belong. Disulfide bonds are also indicated. b, Cys-rich domains of human IGF-1R, IR and EGFR (domains 2 and 4) are aligned based on sequence and structural considerations. Secondary structural elements and disulfide bonds are indicated above the sequences. The dashed bond is only present in IR. Different types of disulfide bonded modules are labelled below the sequences as open, filled or broken lines. Boxed residues show conservation of physico-chemical properties and structurally conserved residues for modules 4-7 are shaded yellow. Residues from EGFR which do not conform to the pattern are shaded grey and the conserved Trp 176 and the semi-conserved Gln 182 are shaded red. This figure was prepared using ALSCRIPT (Barton, G. J., 1993, *Prot. Engineering*, 6:37-40).

Figure 10. Stereo view of a superposition of the L1 (white) and L2 (black) domains. Residues numbers above are for L1 and below for L2. The side chain of Trp 176 which protrudes into the core of L1 is drawn as ball-and-stick.

30

Figure 11. Schematic diagram showing the association of three β -finger motifs. β -strands are drawn as arrows and disulfide bonds as zigzags.

Figure 12. GRASP [Nicolls, A. et al., 1993, *Biophys. J.* 64, 166-170] surface diagram of the L1 domain of IGF-1R shown in a similar view to Figure 8. The

35

N-terminal β -strand is at the top. The mutation L87A [Nakae, J. et al., 1995, J. Biol. Chem. 270, 22017-22022] and four regions (residues 12-15, 34-44, 64-67 and 89-91 of IR) shown to be important in insulin binding to IR [Williams, P. F. et al., 1995, J. Biol. Chem. 270, 3012-3016] correspond to a patch of
 5 residues on the large β -sheet. Residues numbers for IR/IGF-1R are given and residues are coloured according to the magnitude of $K_d(\text{mutant})/K_d(\text{wild type})$, red, > 40 ; orange, 10-40; yellow, 2.5-10; green, < 2.5 ; non-secreting, white; untested, blue. All mutants on the opposite face of the domain do not affect insulin affinity.

10 **Figure 13:** Sequence Alignment of hIGF-1R, hIR and hIRR Ectodomains. Derived by use of the PileUp program in the software package of the Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA. For assignment of homologous 3D structures see Figure 9.

15 **Figure 14:** Sequence Alignment of EGFR, ErbB2, ErbB3 and ErbB4 Ectodomains. Derived by use of the PileUp program in the software package of the Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA. For alignment on the IGF-1R fragment and assignment of homologous
 20 3D structures, see Figure 9.

Figure 15 Sequence Alignment and Classification of the Disulphide-bonded Modules in the Cys-rich domains of IGF-1R, IR, IRR, EGFR, ErbB2, ErbB3 and ErbB4.

25 **Figure 16.** Gel filtration chromatography of insulin receptor ectodomain and MFab complexes. hIR -11 ectodomain dimer (5 - 20 mg) was complexed with MFab derivatives (15-25 mg each) of the anti-hIR antibodies 18-44, 83-7 and 83-14 (Soos et al., 1986). Elution profiles were generated from samples
 30 loaded onto a Superdex S200 column (Pharmacia), connected to a BioLogic chromatography system (Biorad) and monitored at 280 nm. The column was eluted at 0.8 ml/min with 40 mM Tris/150 mM sodium chloride/0.02% sodium azide buffer adjusted to pH 8.0: Profile 0, hIR -11ectodomain, Profile 1, ectodomain mixed with MFab 18-44; Profile 2 , ectodomain mixed with
 35 MFab18-44 and MFab 83-14; Profile 3, ectodomain mixed with MFab 18-44, MFab 83-14 and MFab 83-7. The apparent mass of each complex was

determined from a plot of the following standard proteins: thyroglobulin (660 kDa), ferritin (440 kDa), bovine gammaglobulin (158 kDa), bovine serum albumin (67 kDa), chicken ovalbumin (44 kDa) and equine myoglobin (17 kDa).

5

Figure 17. Micrographs of hIR and hIGF-1R ectodomains. (a) Undecorated hIR ectodomain dimer stained with methylamine tungstate showing parallel bars. (b) Undecorated hIR ectodomain dimer stained with uranyl formate, showing well-spaced parallel bars corresponding to the cartoon below. (c) Undecorated hIGF-1R ectodomain dimer stained with uranyl formate. Magnification bars for (a), (b) and (c) 50nm.

10

Figure 18. Micrographs of hIR and hIGF-1R ectodomains. (a) Thinly stained region of undecorated hIR ectodomain dimers in uranyl formate, showing U-shaped particles (circled) as well as parallel bars as in the cartoon below. (b) Undecorated hIGF-1R ectodomain dimer under similar staining conditions. Magnification bars 50 nm.

15

Figure 19. hIR ectodomain dimer complexed with MFab 83-7 and stained with KPT. Three projections can be recognised: circled particles have the Fab arms displaced either clockwise as in the cartoon below left, or anticlockwise as in the cartoon below middle; arrowed particles have the Fab arms in a central position, cartoon below right. Magnification bar 50 nm.

20

Figure 20. hIR ectodomain dimer complexed with MFab 83-7 and stained with uranyl formate showing the parallel bar structure in particles having the Fab arms displaced (circled). Magnification bar 50 nm.

25

Figure 21. (a) hIR ectodomain dimer complexed with MFab 83-14 stained with potassium phosphotungstate, showing Fab arms attached near the bottom of U-shaped particles (circled). The corresponding cartoon is shown below left. (b) hIR ectodomain dimer complexed with MFab 83-14 stained with uranyl acetate, showing both the view described above (circled) and the parallel-bar view with diagonally projecting Fab arms (arrowed), as in the cartoon below right. Magnification bars 50 nm.

30

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Figure 22 . Double complex of hIR ectodomain dimer with MFabs 83-7 and 18-44 showing particles of complex shape (circled) with four Fab arms attached, consistent with the cartoon below. Magnification bar 50 nm.

- 5 **Figure 23.** Images of hIR ectodomain dimer co-complexed with MFabs 83-7, 83-14 and 18-44 showing examples of complex particles (circled) where it is possible to identify that there are more than four MFabs bound to the dimeric central region. Magnification bar 50 nm.
- 10 **Figure 24.** Schematic illustrating the proposed model of the hIR ectodomain dimer. The dimensions of the molecular envelope are as shown in the diagram, as is the position of the two-fold axis.

Detailed Description of the Invention

- 15 We describe herein the expression, purification, and crystallization of a recombinant IGF-1R fragment (residues 1-462) containing the L1-cysteine-rich-L2 region of the ectodomain. The selected truncation position is just downstream of the exon 6/exon 7 junction (Abbott, A. M., et al., 1992, *J Biol Chem.*, 267:10759-10763) and occurs at a position where the sequences of the
- 20 IR and EGFR families diverge markedly (Ward, C. W., et al., 1995, *Proteins: Struct., Funct., Genet.* 22:141-153; Lax, I., et al., 1988, *Molec. Cellul. Biol.* 8:1970-1978) suggesting it represents a domain boundary. To limit the effects of glycosylation, the IGF-1R fragment was expressed in Lec8 cells, a glycosylation mutant of Chinese hamster ovary (CHO) cells, whose defined
- 25 glycosylation defect produces N-linked oligosaccharides truncated at N-acetyl glucosamine residues distal to mannose residues (Stanley, P. 1989, *Molec. Cellul. Biol.* 9:377-383). Such an approach has facilitated glycoprotein crystallization (Davis, S. J., et al., 1993, *Protein Eng.* 6:229-232; Liu, J., et al., 1996, *J. Biol. Chem.* 271:33639-33646).

- 30 The IGF-1R construct described herein included a c-myc peptide tag (Hoogenboom, H. R., et al., 1991, *Nucleic Acids Res.* 19:4133-4137) that is recognised by the Mab 9E10 (Evan, G. I., et al., 1985, *Mol. Cell. Biol.* 5:3610-3616) enabling the expressed product to be purified by peptide elution from an antibody affinity column followed by gel filtration over Superdex S200.
- 35 The purified proteins crystallized under a sparse matrix screen (Jancarik, J. & Kim, S.-H., 1991, *J. Appl. Cryst.* 24:409-411) but the crystals were of variable

quality, with the best diffracting to 3.0-3.5Å. Isocratic gradient elution by anion-exchange chromatography yielded protein that was less heterogenous and gave crystals of sufficient quality to determine the structure of the first three domains of the human IGF-1R.

5 The IGF-1R fragment consisted of residues 1-462 of IGF-1R linked via an enterokinase-cleavable pentapeptide sequence to an eleven residue c-myc peptide tag at the C-terminal end. The fragment was expressed in Lec8 cells by continuous media perfusion in a bioreactor using porous carrier disks. It was secreted into the culture medium and purified by peptide elution from
10 an anti-c-myc antibody column followed by Superdex S200 gel filtration. The receptor fragment bound two anti-IGF-1R monoclonal antibodies, 24-31 and 24-60, which recognize conformational epitopes, but could not be shown to bind IGF-1 or IGF-2. Crystals of variable quality were grown as rhombic
15 prisms in 1.7 M ammonium sulfate at pH 7.5 with the best diffracting to 3.0-3.5 Å. Further purification by isocratic elution on an anion-exchange column gave protein which produced better quality crystals, diffracting to 2.6 Å, that were suitable for X-ray structure determination.

 The structure of this fragment (IGF-1R residues 1-462; L1-cys rich-L2domains) has been determined to 2.6 Å resolution by X-ray diffraction. The
20 L domains each adopt a compact shape consisting of a single stranded right-handed β-helix. The cys-rich region is composed of eight disulphide-bonded modules, seven of which form a rod-shaped domain with modules associated in a novel manner. At the centre of this reasonably extended structure is a space, bounded by all three domains, and of sufficient size to accommodate a
25 ligand molecule. Functional studies on IGF-1R and other members of the insulin receptor family show that the regions primarily responsible for hormone-binding map to this central site. Thus this structure gives a first view of how members of the insulin receptor family might interact with their ligands.

30 Another group has reported the crystallization of a related receptor, the EGFR in a complex with its ligand EGF (Weber, W., et al., 1994, J Chromat. 679:181-189). However difficulties were encountered with these crystals which diffracted to only 6 Å, insufficient for the determination of an atomic resolution structure of this complex (Weber, W., et al., 1994, J
35 Chromat 679:181-189) or the generation of accurate models of structurally related receptor domains such as IGF-1R and IR by homology modelling.

The present inventors have applied the same process to the IR and generated a fragment (residues 1-485) that covers the first three domains of the IR. This fragment has been expressed in transformed Lec8 cells, purified, and crystallized by similar methodologies to yield crystals suitable for X-ray diffraction.

The present inventors have therefore developed 3D structural information about cytokine receptors to enable a more accurate understanding of how the binding of ligand leads to signal transduction. Such information provides a rational basis for the development of antagonists or agonists for specific therapeutic applications, something that heretofore could not have been predicted *de novo* from available sequence data.

The precise mechanisms underlying the binding of agonists and antagonists to the IGF-1 receptor site are not fully clarified. However, the binding of the agonists or antagonists to the receptor site, preferably with an affinity in the order of 10^{-8} M or higher, is understood to arise from enhanced stereochemical complementarity, relative to naturally occurring IGF-1 ligands.

Such stereochemical complementarity, pursuant to the present invention, is characteristic of a molecule that matches intra-site surface residues lining the groove of the receptor site as enumerated by the coordinates set out in Figure 1. The residues lining the groove are depicted in Figure 2. Substances which are complementary to the shape of the receptor site characterised by amino acids positioned at atomic coordinates set out in Figure 1 may be able to bind to the receptor site and, when the binding is sufficiently strong, substantially prohibit binding of the naturally occurring ligands to the site.

It will be appreciated that it is not necessary that the complementarity between agonists or antagonists and the receptor site extend over all residues lining the groove in order to inhibit binding of the natural ligand. Accordingly, agonists or antagonists which bind to a portion of the residues lining the groove are encompassed by the present invention.

In general, the design of a molecule possessing stereochemical complementarity can be accomplished by means of techniques that optimize, either chemically or geometrically, the "fit" between a molecule and a target receptor. Known techniques of this sort are reviewed by Sheridan and Venkataraghavan, *Acc. Chem Res.* 1987 20 322; Goodford, *J. Med. Chem.*

1984 27 557; Beddell, Chem. Soc. Reviews 1985, 279; Hol, Angew. Chem. 1986 25 767 and Verlinde C.L.M.J & Hol, W.G.J. Structure 1994, 2, 577, the respective contents of which are hereby incorporated by reference. See also Blundell et al., Nature 1987 326 347 (drug development based on information
5 regarding receptor structure).

Thus, there are two preferred approaches to designing a molecule, according to the present invention, that complements the shape of IGF-1R or a related receptor molecule. By the geometric approach, the number of internal degrees of freedom (and the corresponding local minima in the
10 molecular conformation space) is reduced by considering only the geometric (hard-sphere) interactions of two rigid bodies, where one body (the active site) contains "pockets" or "grooves" that form binding sites for the second body (the complementing molecule, as ligand). The second preferred approach entails an assessment of the interaction of respective chemical
15 groups ("probes") with the active site at sample positions within and around the site, resulting in an array of energy values from which three-dimensional contour surfaces at selected energy levels can be generated.

The geometric approach is illustrated by Kuntz et al., J. Mol. Biol. 1982 161 269, the contents of which are hereby incorporated by reference,
20 whose algorithm for ligand design is implemented in a commercial software package distributed by the Regents of the University of California and further described in a document, provided by the distributor, which is entitled "Overview of the DOCK Package, Version 1.0," the contents of which are hereby incorporated by reference. Pursuant to the Kuntz algorithm, the
25 shape of the cavity represented by the IGF-R1 site is defined as a series of overlapping spheres of different radii. One or more extant data bases of crystallographic data, such as the Cambridge Structural Database System maintained by Cambridge University (University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, U.K.) and the Protein Data Bank
30 maintained by Brookhaven National Laboratory (Chemistry Dept. Upton, NY 11973, U.S.A.), is then searched for molecules which approximate the shape thus defined.

Molecules identified in this way, on the basis of geometric parameters, can then be modified to satisfy criteria associated with chemical
35 complementarity, such as hydrogen bonding, ionic interactions and Van der Waals interactions.

The chemical-probe approach to ligand design is described, for example, by Goodford, J. Med. Chem. 1985 28 849, the contents of which are hereby incorporated by reference, and is implemented in several commercial software packages, such as GRID (product of Molecular Discovery Ltd., West
5 Way House, Elms Parade, Oxford OX2 9LL, U.K.). pursuant to this approach, the chemical prerequisites for a site-complementing molecule are identified at the outset, by probing the active site (as represented via the atomic coordinates shown in Fig. 1) with different chemical probes, e.g., water, a methyl group, an amine nitrogen, a carboxyl oxygen, and a hydroxyl.
10 Favored sites for interaction between the active site and each probe are thus determined, and from the resulting three-dimensional pattern of such sites a putative complementary molecule can be generated.

The chemical-probe approach is especially useful in defining variants of a molecule known to bind the target receptor. Accordingly,
15 crystallographic analysis of IGF-1 bound to the receptor site may provide useful information regarding the interaction between the archetype ligand and the active site of interest.

A further use of the structure of IGF-1R fragment described here is in facilitating structure determination of a related protein such as a larger
20 fragment of this receptor, another member of the insulin receptor family or a member of the EGF receptor family. This new structure could be either alone or in complex with its ligand. For crystallographic analysis this is achieved using the method of molecular replacement (Brunger, Meth. Enzym. 1997 276 558-580, Navaza and Saludjian, *ibid.* 581-594, Tong and Rossmann, *ibid.* 594-
25 611, Bentley, *ibid.* 611-619) in a program such as XPLOR. In this procedure diffraction data is collected from a crystalline protein of unknown structure. A transform of these data (Patterson function) is compared with a Patterson function calculated from a known structure. Firstly, the one Patterson function is rotated on the other to determine the correct orientation of the
30 unknown molecule in the crystal. The translation function is then calculated to determine the location of the molecule with respect to the crystal axes. Once the molecule has been correctly positioned in the unit cell initial phases for the experimental data may be calculated. These phases are necessary for calculation of an electron density map from which structural
35 differences may be observed and for refinement of the structure. Due to limitations in the method the search molecule must be structurally related to

that which is to be determined. However it is sufficient for only part of the unknown structure (e.g. < 50%) to be similar to the search molecule. Thus the three dimensional structure of IGF-1R residues 1-462 may be used to solve structures consisting of related receptors, enabling a program of drug design as outlined above.

In summary, the general principles of receptor-based drug design can be applied by persons skilled in the art, using the crystallographic results presented above, to produce agonists or antagonists of IGF-1R or other related receptors, having sufficient stereochemical complementarity to exhibit high affinity binding to the receptor site.

The present invention is further described below with reference to the following, non-limiting examples.

EXAMPLE 1

Expression, Purification and Crystalization of the IGF-1R Fragment

Several factors hamper macromolecular crystallization including sample selection, purity, stability, solubility (McPherson, A., et al., 1995, Structure 3:759-768); Gilliland, G. L., & Ladner, J. E., 1996, Curr. Opin. Struct. Biol. 6:595-603), and the nature and extent of glycosylation (Davis, S. J., et al., 1993, Protein Eng. 6:229-232). Initial attempts to obtain structural data from soluble IGF-1R ectodomain (residues 1-906) protein, expressed in Lec8 cells (Stanley, P. 1989, Molec. Cellul. Biol. 9:377-383) and purified by affinity chromatography, produced large, well-formed crystals (1.0 mm x 0.2 mm x 0.2 mm) which gave no discernable X-ray diffraction pattern (unpublished data). Similar difficulties have been encountered with crystals of the structurally related epidermal growth factor receptor (EGFR) ectodomain which diffracted to only 6 Å, insufficient for the determination of an atomic resolution structure (Weber, W. et al., 1994, J Chromat 679:181-189). This prompted us to search for a fragment of IGF-1R that was more amenable to X-ray crystallographic studies.

The fragment expressed (residues 1-462) comprises the L1-cysteine-rich-L2 region of the ectodomain. The selected truncation position at Val462 is four residues downstream of the exon 6/exon 7 junction (Abbott, A. M., et al., 1992, J Biol Chem. 267:10759-10763) and occurs at a position where the sequences of the IR and the structurally related EGFR families diverge markedly (Lax, I., et al., 1988, Molec Cell Biol. 8:1970-1978; Ward, C. W., et

- al., 1995, *Proteins: Struct., Funct., Genet.* 22:141-153), suggesting it represents a domain boundary. The expression strategy included use of the pEE14 vector (Bebbington, C. R. & Hentschel, C. C. G., 1987, In: Glover, D. M., ed. *DNA Cloning*. Academic Press, San Diego. Vol 3, p163) in
- 5 glycosidase-defective Lec8 cells (Stanley, P., 1989, *Molec. Cellul. Biol.* 9:377-383), which produce N-linked oligosaccharides lacking the terminal galactose and N-acetylneuraminic acid residues (Davis, S. J., et al., 1993, *Protein Eng.* 6:229-232; Liu, T., et al., 1996, *J Biol Chem* 271:33639-33646.). The construct contained a C-terminal c-myc affinity tag (Hoogenboom, H. R., et al., 1991,
- 10 *Nucl Acids Res.* 19:4133-4137), which facilitated immunoaffinity purification by specific peptide elution and avoided aggressive purification conditions. These procedures yielded protein which readily crystallized after a gel filtration polish. This provided a general protocol to enhance crystallisation prospects for labile, multidomain glycoproteins.
- 15 The structure of this fragment is of considerable interest since it contains the major determinants governing insulin and IGF-1 binding specificity (Gustafson, T. A. & Rutter, W. J., 1990, *J. Biol. Chem.* 265:18663-18667; Andersen, A. S., et al., 1990, *Biochemistry*, 29:7363-7366; Schumacher, R., et al., 1991, *J. Biol. Chem.* 266:19288-19295; Schumacher,
- 20 R., et al., 1993, *J. Biol. Chem.* 268:1087-1094; Schäffer, L., et al., 1993, *J. Biol. Chem.* 268:3044-3047; Williams, P. F., et al., 1995, , *J. Biol. Chem.* 270:3012-3016) and is very similar to an IGF-1R fragment (residues 1-486) reported to act as a strong dominant negative for several growth functions and which induces apoptosis of tumour cells in vivo (D'Ambrosio, C., et al., 1996,
- 25 *Cancer Res.* 56:4013-4020).
- The expression plasmid pEE14/IGF-1R/462 was constructed by inserting the oligonucleotide cassette:

AatII

30 5' GACGTC GACGATGACGATAAG GAACAAAACTCATC

D V D D D D K E Q K L I

(EK cleavage) (c-myc tail)

S E E D L N (Stop)

TCAGAAGAGGATCTGAAT TAGAATTC GACGTC 3'

35 *EcoRI AatII*

encoding an enterokinase cleavage site, c-myc epitope tag (Hoogenboom, H. R., et al., 1991, *Nucleic acids Res.* 19:4133-4137) and stop codon into the AatII site (within codon 462) of IGF-1 receptor cDNA in the mammalian expression vector pECE (Ebina, Y., et al., 1985, *Cell*, 40:747-758; kindly
 5 supplied by W. J. Rutter, UCSF, USA), and introducing the DNA comprising the 5' 1521 bp of the cDNA (Ullrich, A., et al., 1986, *EMBO J.* 5:2503-2512) ligated to the oligonucleotide cassette into the EcoRI site of the mammalian plasmid expression vector pEE14 (Bebbington, C. R. & Hentschel, C. C. G., 1987, In: Glover, D. M., ed. *DNA Cloning*. Academic Press, San Diego. Vol 3,
 10 p163; Celltech Ltd., UK). Plasmid pEE14/IGF-1R/462 was transfected into Lec8 mutant CHO cells (Stanley, P. 1989, *Molec. Cellul. Biol.* 9:377-383) obtained from the American Tissue Culture Collection (CRL:1737) using Lipofectin (Gibco-BRL). Cell lines were maintained after transfection in glutamine-free medium (Glasgow modification of Eagle's medium (GMEM;
 15 ICN Biomedicals, Australia) and 10% dialysed FCS (Sigma, Australia) containing 25 μ M methionine sulfoximine (MSX; Sigma, Australia) as described (Bebbington, C. R. & Hentschel, C. C. G., 1987, In: Glover, D. M., ed. *DNA Cloning*. Academic Press, San Diego. Vol 3, p163). Transfectants were screened for protein expression by Western blotting and sandwich
 20 enzyme-linked immunosorbant assay (ELISA) (Cosgrove, L., et al., 1995,) using monoclonal antibody (Mab) 9E10 (Evan et al., 1985) as the capture antibody and either biotinylated anti-IGF-1R Mab 24-60 or 24-31 for detection (Soos et al., 1992; gifts from Ken Siddle, University of Cambridge, UK). Large-scale cultivation of selected clones expressing IGF-1R/462 was
 25 carried out in a Celligen Plus bioreactor (New Brunswick Scientific, USA) containing 70 g Fibra-Cel Disks (Sterilin, UK) as carriers in a 1.25 L working volume. Continuous perfusion culture using GMEM medium supplemented with non-essential amino acids, nucleosides, 25 μ M MSX and 10% FCS was maintained for 1 to 2 weeks followed by the more enriched DMEM/F12
 30 without glutamine, with the same supplementation for the next 4-5 weeks. The fermentation production run was carried out three times under similar conditions and resulted in an estimated overall yield of 50 mg of receptor protein from 430 L of harvested medium. Cell growth was poor during the initial stages of the fermentation when GMEM medium was employed, but
 35 improved dramatically following the switch to the more enriched medium. Target protein productivity was essentially constant during the period from

~100 to 700 h of the 760 h fermentation, as measured by ELISA using Mab 9E10 as the capture antibody and biotinylated Mab 24-31 as the developing antibody.

Soluble IGF-1R/462 protein was recovered from harvested
 5 fermentation medium by affinity chromatography on columns prepared by coupling Mab 9E10 to divinyl sulphone-activated agarose beads (Mini Leak; Kem En Tec, Denmark) as recommended by the manufacturer. Mini-Leak Low and Medium affinity columns with antibody loadings of 1.5-4.5 mg/ml of hydrated matrix were obtained, with the loading range of 2.5-3 mg/ml giving
 10 optimal performance (data not shown). Mab 9E10 was produced by growing hybridoma cells (American Tissue Culture Collection) in serum-free medium in the Celligen Plus bioreactor and recovering the secreted antibody (4 g) using protein A glass beads (Prosep-A, Bioprocessing Limited, USA). Harvested culture medium containing IGF-1R/462 protein was adjusted to pH
 15 8.0 with Tris-HCl (Sigma), made 0.02% (w/v) in sodium azide and passed at 3-5 ml/min over 50 ml Mab 9E10 antibody columns at 4° C. Bound protein was recovered by recycling a solution of 2-10 mg of the undecamer c-myc peptide EQKLISEEDLN (Hoogenboom et al., 1991) in 20 ml of Tris-buffered saline containing 0.02% sodium azide (TBSA). Between 65% and 75% of the
 20 product was recovered from the medium as estimated by ELISA, with a further 15-25% being recovered by a second pass over the columns. Peptide recirculation (~10 times) through the column eluted bound protein more efficiently than a single, slower elution. Residual bound protein was eluted with sodium citrate buffer at pH 3.0 into 1 M Tris HCl pH 8.0 to neutralize
 25 the eluant, and columns were re-equilibrated with TBSA.

Gel filtration over Superdex S200 (Pharmacia, Sweden), of affinity-purified material showed a dominant protein peak at ~63 kDa, together with a smaller quantity of aggregated protein (Figure 3a). The peak protein migrated primarily as two closely spaced bands on reduced , sodium dodecyl
 30 sulfate polyacrylamide gel electrophoresis (SDS-PAGE; Figure 3b), reacted positively in the ELISA with both Mab 24-60 and Mab 24-31, and gave a single sequence corresponding to the N-terminal 14 residues of IGF-1R. No binding of IGF-1 or IGF-2 could be detected in the solid plate binding assay (Cosgrove et al., 1995, Protein Express Purif. 6:789-798). The IGF-1R/462
 35 fragment was further purified by ion-exchange chromatography on Resource Q (Pharmacia, Sweden). Using shallow salt gradients, protein enriched in the

slowest migrating SDS-PAGE band was obtained (data not shown), which formed relatively large, well-formed crystals (see below). Isoelectric focusing showed the presence of one major and two minor isoforms. Protein purified on Resource Q with an isocratic elution step of 0.14 M NaCl in 20 mM TrisCl at pH 8.0 (fraction 2, Figure 4) showed less heterogeneity on isoelectric focusing (Figure 4 inset) and SDS-PAGE (data not shown) and produced crystals of sufficient quality for structure determination (see below).

Crystals were grown by the hanging drop vapour diffusion method using purified protein concentrated in Centricon 10 concentrators (Amicon Inc, USA) to 5-10 mg/ml in 10-20 mM Tris-HCl pH 8.0 and 0.02% (w/v) azide, or 100 mM ammonium sulfate and 0.02% (w/v) azide. A search for crystallization conditions was performed initially using the factorial screen (Jancarik, J. & Kim, S.-H., 1991, J Appl Cryst 24:409-411) and subsequently optimised. Crystals were examined on an M18XHF rotating anode generator (Siemens, Germany) equipped with Franks mirrors (MSC, USA) and RAXIS IIC and IV image plate detectors (Rigaku, Japan).

From the initial crystallization screen of this protein, crystals of about 0.1 mm in size grew in one week. Upon refining conditions, crystals of up to 0.6 x 0.4 x 0.4 mm could be grown from a solution of 1.7-2.0 M ammonium sulfate, 0.1 M HEPES pH 7.5. The crystals varied considerably in shape and diffraction quality, growing predominantly as rhombic prisms with a length to width ratio of up to 5:1, but sometimes as rhombic bipyramids, the latter form being favoured when using material which had been eluted from the Mab 9E10 column at pH 3.0. Each crystal showed a minor imperfection in the form of very faint lines from the centre to the vertices. Protein from dissolved crystals did not appear to be different from the protein stock solution when run on an isoelectric focusing gel. Upon X-ray examination, the crystals diffracted to 3.0-4.0 Å and were found to belong to the space group $P2_12_12_1$ with $a = 76.8$ Å, $b = 99.0$ Å, $c = 119.6$ Å. In the diffraction pattern, the crystal variability noted above was manifest as a large (1-2°) and anisotropic mosaic spread, with concomitant variation in resolution. To improve the quality of the crystals, they were grown in the presence of various additives or were recrystallized. These methods failed to substantially improve the crystal quality although bigger crystals were obtained by recrystallization. The variability in crystal quality appeared to be due to protein heterogeneity, as demonstrated by the observation that more

highly purified protein, eluted isocratically from the Resource Q column and showing one major band on isoelectric focusing (Figure 4 inset), produced crystals of sufficient quality for structure determination. These crystals diffracted to 2.6 Å resolution with cell dimensions, $a = 77.0$ Å, $b = 99.5$ Å, $c = 120.1$ Å and mosaic spread of 0.5°. Heavy metal derivatives of the IGF-1R/462 crystals have been obtained and are leading to the determination of an atomic resolution structure of this fragment, which contains the L1, cysteine-rich and L2 domains of human IGF-1R.

EXAMPLE 2

10 Expression, Purification and Crystalization of the IR Fragment

A similar strategy was adopted for the human insulin receptor. The fragment expressed (residues 1-485) comprises the L1-cysteine-rich-L2 region of the IR ectodomain but extends 13 residues further before the attachment of the 17 residue EK cleavage site linker and c-myc tail. The selected truncation position corresponds to a unique and convenient Bgl II restriction site. The expression strategy was also based on the pEE14 expression vector in glycosidase-defective Lec8 cells and use of a C-terminal c-myc affinity tag for immunoaffinity purification by specific peptide elution. These procedures yielded IR protein which readily crystallized after a gel filtration polish.

20 The expression plasmid pHIR485 was constructed by ligating the double-stranded oligonucleotide cassette:

| | | | |
|----|--|------------|--------------|
| | <i>Bgl</i> II | | <i>Xba</i> I |
| 25 | 5' AGATC TCCGACGATGACGATAAG GAACAAAACATCTCAGAAGAGGATCTGAAT TAG TCTAGA 3' | | |
| | K I S D D D D K E Q K L I S E E D L N | | |
| | EK cleavage | c-myc tail | Stop |

encoding an enterokinase cleavage site, c-myc epitope tag (Hoogenboom, H. R., et al., 1991, Nucleic acids Res. 19:4133-4137) and stop codon, to the larger 11.1 kilobasepair Bgl II / Xba I fragment isolated from digestion of the mammalian expression plasmid pEH3 (a derivative of the mammalian plasmid expression vector pEE14 [Bebbington, C. R. & Hentschel, C. C. G., 1987, In: Glover, D. M., ed. DNA Cloning. Academic Press. San Diego. Vol 3, p163; Celltech Ltd., UK] which holds the entire coding sequence of human insulin receptor within a Hind III/Xba I fragment). Lec8 mutant CHO cells

(Stanley, P. 1989, *Molec. Cellul. Biol.* 9:377-383) obtained from the American Tissue Culture Collection (CRL:1737) were transfected with pHIR485 using Lipofectamine (Gibco-BRL). Cell lines were maintained after transfection in glutamine-free medium (Glasgow modification of Eagle's medium - GMEM; 5 ICN Biomedicals, Australia) and 10% dialysed FCS (Sigma, Australia) containing 25 μ M methionine sulfoximine (MSX; Sigma, Australia) as described (Bebbington, C. R. & Hentschel, C. C. G., 1987, In: Glover, D. M., ed. *DNA Cloning*. Academic Press, San Diego. Vol 3, p163). Transfectants were screened for protein expression by Western blotting and sandwich 10 enzyme-linked immunosorbant assay (ELISA) (Cosgrove, L., et al., 1995,) using anti-hIR (Mab) 83.7 as the primary antibody and biotinylated monoclonal antibody (Mab) 9E10 (Evan et al., 1985) for detection (Soos et al., 1986; gifts from Ken Siddle, University of Cambridge, UK).

Large-scale cultivation of selected clones expressing IR/485 was carried out 15 in a Celligen Plus bioreactor (New Brunswick Scientific, USA) containing 70 g Fibra-Cel Disks (Sterilin, UK) as carriers in a 1.25 L working volume. Continuous perfusion culture was carried out using DMEM/F12 without glutamine medium (ICN), supplemented with non-essential amino acids, nucleosides, 25 μ M MSX and 5 - 10% FCS and resulted in an estimated 20 overall yield of 115 mg of receptor protein from 165 L of harvested medium. Target protein productivity was essentially constant during the fermentation, as measured by ELISA.

Soluble IR/485 protein was recovered from harvested fermentation medium by affinity chromatography on columns of Mab 9E10 essentially as 25 described in Example 1. Between 92 -98% of the product was recovered from the medium by this affinity-chromatography step, as estimated by ELISA.

Gel filtration over Superdex 200 (Pharmacia, Sweden), of the affinity-purified material at 1mg/ml produced a dominant protein peak at apparent mass \sim 140 kDa (Figure 5a - interpreted as dimer), whereas a peak at apparent 30 mass \sim 85 kDa was obtained (Figure 5b - interpreted as monomer) at 0.02 mg/ml. The protein migrated as a single broad band of apparent molecular mass \sim 78 kDa (reduced- lane A) or \sim 68 kDa (non-reduced - lane B) on sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE; Figure 6a) The IR/485 fragment reacted positively in the ELISA with Mab 83- 35 7, gave a single sequence corresponding to the N-terminal 10 residues of IR, showing several isoforms on isoelectric focussing from pI 6.0 - 6.8 (Figure

6b). Crystallisation screening trials of the fragment produced crystals too small for X-ray diffraction studies. The fragment was further purified by ion-exchange chromatography on Uno Q (BioRad, USA), using stepwise isocratic elution with incremental changes in salt concentrations (Figure 7). Fractions
 5 A and D were each enriched in a component isoform from the ladder of isoforms present in the unfractionated mixture (Figure 6b). Both these fractions produced crystals, whereas no crystals were obtained from fractions B and C.

Crystals were grown by the hanging drop vapour diffusion method
 10 using purified protein concentrated in Centricon 10 concentrators (Amicon Inc, USA) to 5-10 mg/ml in 10mM Tris-HCl pH 8.0 and 0.02% (w/v) azide. A search for crystallization conditions was performed initially using the factorial screen (Jancarik, J. & Kim, S.-H., 1991, J Appl Cryst 24:409-411) and subsequently optimised. Crystals were examined on an M18XHF rotating
 15 anode generator (Siemens, Germany) equipped with Franks mirrors (MSC, USA) and an RAXIS IIC image plate detector (Rigaku, Japan).

From the initial crystallization screen of this protein fraction D fine needles grew in about one week. In further experiments, crystals of up to 0.04 x 0.04 x 0.2 mm could be grown from a solution of 1.9-2.0 M ammonium
 20 sulfate, 2% PEG 400, 0.1 M HEPES pH 7.5. Upon X-ray examination, the crystals diffracted to 4 Å and were found to belong to the space group $P2_12_12_1$ with $a = 103.2$ Å, $b = 130.0$ Å, $c = 161.6$ Å. Despite their small size these crystals diffracted sufficiently well to allow collection of a low resolution data set. Further purification of the protein and refinement of crystallisation
 25 conditions should yield larger crystals, providing data to determine the structure of this fragment at medium resolution or better.

EXAMPLE 3

Structure of the IGF-1R/1-462

Crystals were cryo-cooled to -170°C in a mother liquor containing 20%
 30 glycerol, 2.2 M ammonium sulfate and 100 mM Tris at pH 8.0. Native and derivative diffraction data were recorded on Rigaku RAXIS IIC or IV area detectors using copper K α radiation from a Siemens rotating anode generator with Yale/MSC mirroroptics. The space group was $P2_12_12_1$ with $a = 77.39$ Å, $b = 99.72$ Å, and $c = 120.29$ Å. Data were reduced using DENZO and
 35 SCALEPACK (Otwinowski, Z. & Minor, W., 1996, *Methods in Enzymology* 276:307-326). Diffraction was notably anisotropic for all crystals examined.

Phasing by multiple isomorphous replacement(MIR) was performed with PROTEIN (Steigeman, W. Dissertation (Technical Univ. Munich, 1974) using anomalous scattering for both UO₂ and PIP derivatives. Statistics for data collection and phasing are given in Table 1. In the initial MIR map regions of protein and solvent could clearly be seen but the path of the polypeptide was by no means obvious. That map was subject to solvent flattening and histogram matching in DM (Cowtan, K., 1994, Joint CCP4 and ESF-EACBM newslett. Protein Crystallogr. 31:34-38). The structure was traced and rebuilt using O (Jones, T. A., et al., 1991, Acta Crystallogr. A47:110-119) and refined with X-PLOR 3.851 (Brunger, A. T., 1996, X-PLOR ReferenceManual 3.851, Yale Univ., New Haven, CT). After 5 rounds of rebuilding and energy minimisation the R-factor dropped to 0.279 and R_{free} = 0.359 for data 7-2.6 Å resolution. The current model contains 458 amino acids and 3 N-linked carbohydrates but no solvent molecules. For residues with B(Ca) > 70 Å² atomic positions are less reliable (37-42, 155-159, 305, 336-341, 404-406, 453-458). There is weak electron density for residues 459-461 but the c-myc tail appears completely disordered.

The 1-462 fragment consists of the N-terminal three domains of IGF-1R (L1, cys-rich, L2) and contains regions of the molecule which dictate ligand specificity (17-23). The molecule adopts a reasonably extended structure (approximately 40 x 48 x 105 Å) with domain 2 (cys-rich region) making contact along the length of domain 1 (L1) but very little contact with the third domain (L2) (see Figure 8). This leaves a space at the centre of the molecule of approximately 24 Å x 24 Å x 24 Å which is bounded on three sides by the three domains of the molecule. The space is of sufficient size to accommodate the ligand, IGF-1.

The L domains

Each of the L domains (residues 1-150 and 300-460) adopt a compact shape (24 x 32 x 37 Å) consisting of a single-stranded right handed β-helix and capped on the ends by short α-helices and disulfide bonds. The body of the domain looks like a loaf of bread with the base formed from a flat six-stranded β-sheet, 5 residues long and the sides being β-sheets three residues long (Figures 8 & 9). The top is irregular but in places is similar for the two domains. The two domains are superposable with an rms deviation in Ca positions of 1.6 Å for 109 atoms (Figure 10). Although this fold is reminiscent of other β-helix proteins it is much simpler and smaller with very few

elaborations and thus it represents a new superfamily of domains. One notable difference between the two domains is that the indole ring of Trp 176 from the cys-rich region (Figure 9b) is inserted into the hydrophobic core of L1 and the C-terminal helix is only vestigial (Figure 8). For the insulin

5 receptor family the sequence motif of residues which form the Trp pocket in L1 does not occur in L2 (Figure 9a). However in the EGF receptor, which has an additional cys-rich region after the L2 domain (14, 15), the pocket motif can be found in both L domains and the Trp is conserved in both cys-rich regions (Figure 9b).

10 The repetitive nature of the β -helix is reflected in the sequence and the first five turns were correctly identified by Bajaj, M., et al. (1987, *Biochim.Biophys. Acta* 916:220-226), the conserved Gly residues being found in turns making one bottom edge of the domain. However, their conclusions about the fold were incorrect. The "helix-like" repeat is actually a pair of

15 bends at the top edge of the domain. In their Motif V, the Gly is not in a bend but is followed by the insertion of a conserved loop of 7-8 residues (see Figure 9a). Glycine is structurally important in the Gly bends as mutation of these residues compromises folding of the receptor [van der Vorm, E.R., et al., 1992, *J. Biol. Chem.* 267, 66-71; Wertheimer, E. et al., 1994, *J. Biol. Chem.*

20 269, 7587-7592].

Upon comparing the L domains with other right-handed β -helix structures such as pectate lyase (Yoder, M. D., et al., 1993, *Structure*, 1:241-251-1507) and the p22 tailspike protein (Steinbacher, S., et al., 1997, *J.Mol. Biol.* 267:865-880) there are some striking similarities as well as differences.

25 In all cases the ends of the domain are capped by α -helices but the L domains also have a disulphide bond at each end to hold the termini. The other β -helix domains are considerably longer and have significant twist to their sheets while the L domains have flat sheets. Although the sizes of the helix repeats are similar (here 24-25 residues vs 22-23 for pectate lyase) the cross-

30 sections are quite different. The L domains have a rectangular cross-section while pectate lyase and p22 tailspike protein are V-shaped and have many, and sometimes quite large, insertions (Yoder, M. D., et al., 1993, *Structure*, 1:241-251-1507; Steinbacher, S., et al., 1997, *J.Mol. Biol.* 267:865-880). In the hydrophobic core a common feature is the stacking of aliphatic residues

35 from successive turns of the β -helix and near the C-terminus of each L domain there is also a short Asn ladder, reminiscent of the long Asn ladder

observed in pectate lyase (Yoder, M. D., et al., 1993, Structure 1:241-251-1507). On the opposite side of the L domains the Gly bend as well as the two bends and sheet preceding it have no counterpart in the other β -helix domains. Thus although the L domains are built on similar principles to the other β -helix domains they constitute a separate superfamily.

The cys-rich domain

The cys-rich domain is composed of eight disulfide-bonded modules (Figure 9b), the first of which sits at the end of L1 while the remainder make a curved rod running diagonally across L1 and reaching to L2 (Figure 8). The strands in modules 2-7 run roughly perpendicular to the axis of the rod in a manner more akin to laminin (Stetefeld, J., et al., 1996, J.Mol.Biol. 257:644-657) than to TNF receptor (Banner, D. W., et al., 1993, Cell, 73:431-445) but the modular arrangement of the cys-rich domain is different to other cys-rich proteins for which structures are known. The first 3 modules of IGF-1R have a common core, containing a pair of disulfide bonds, but show considerable variation in the loops (Figure 9b). The connectivity of these modules is the same as the first half of EGF (Cys 1-3 and 2-4) but their structures do not appear to be closely related to any member of the EGF family. Modules 4 to 7 have a different motif, β -finger, and best match residues 2152-2168 of fibrillin (Dowling, A. K., et al., 1996, Cell, 85:597-605). Each is composed of three polypeptide strands, the first and third being disulfide bonded and the latter two forming a β -ribbon. The β -ribbon of each β -finger module lines up antiparallel to form a tightly twisted 8-stranded β -sheet (Figures 8 and 11). Module 6 deviates from the common pattern with the first segment being replaced by an α -helix followed by a large loop that is likely to have a role in ligand binding (see below). As module 5 is most similar to module 7 it is possible that the four modules arose from serial gene duplications. The final module is a disulfide linked bend of five residues.

The fact that the two major types of cys-rich modules occur separately implies that these are the minimal building blocks of cys-rich domains found in many proteins. Although it can be as short as 16 residues, the motif of modules 4-7 is clearly distinct and capable of forming a regular extended structure. Thus cys-rich domains such as these can be considered as made of repeat units each composed of a small number of modules.

Hormone binding

Attempts have been made to locate the IGF-1 (and insulin) binding site by examining natural (Taylor, S. I., 1992, *Diabetes*, 41:1473-1490) and site-directed mutants (Williams, P. F., et al., 1995, *J. Biol. Chem.* 270:3012-3016; Mynarcik, D. C et al., 1996, *J. Biol. Chem.* 271:2439-2442; Mynarcik, D. C., et al., 1997, *J. Biol. Chem.* 272:2077-2081), chimeric receptors (Andersen, A. S., et al., 1990, *Biochemistry* 29:7363-7366; Gustafson, T. A., & Rutter, W. J., 1990, *J. Biol. Chem.* 265:18663-18667; Schäffer, L., et al., 1993, *J. Biol. Chem.* 268:3044-3047; Schumacher, R., 1993, *J. Biol. Chem.* 268:1087-1094; Kjeldsen, T., et al., 1991, *Proc. Natl Acad. Sci. USA*, 88:4404-4408) and by crosslinking studies (Wedekind, F., et al., 1989, *Biol. Chem Hoppe-Seyler*, 370:251-258; Fabry, M., 1992, *J. Biol. Chem.* 267:8950-8956; Waugh, S. M., et al., 1989, *Biochemistry*, 28:3448-3458; Kurose, T., et al., 1994), *J. Biol. Chem.* 269:29190-29197-34). IGF-1R/IR chimeras not only show which regions of the receptors account for ligand specificity but also provide an efficient means of identifying some parts of the hormone binding site. Paradoxically regions controlling specificity are not the same for insulin and IGF-1. Replacing the first 68 residues of IGF-1R with those of IR confers insulin binding ability on the chimeric IGF-1R (Kjeldsen, T., et al., 1991, *Proc. Natl Acad. Sci. USA*, 88:4404-4408) and replacing residues 198-300 in the cys-rich region of IR with the corresponding residues 191-290 of IGF-1R allows the chimeric receptor to bind IGF-1 (Schäffer, L., et al., 1993, *J. Biol. Chem.* 268:3044-3047). Thus a receptor can be constructed which binds both IGF-1 and insulin with near native affinity. From the structure it is clear that if the hormone bound in the central space it could contact both these regions.

From analysis a series of chimeras examined by Gustafson, T. A., & Rutter, W. J. (*J. Biol. Chem.* 265:18663-18667, 1990) the specificity determinant in the cys-rich region can be limited further to residues 223-274. This region corresponds to modules 4-6 and includes a large and somewhat mobile loop (residues 255-263, mean B[Ca atoms] = 57 Å²) which extends into the central space (see Figure 8). In IR this loop is four residues bigger and is stabilised by an additional disulfide bond (Schäffer, L. & Hansen, P.H., 1996, *Exp. Clin. Endocrinol. Diabetes*, 104: Suppl. 2, 89). The larger loop of IR may serve to exclude IGF-1 from the hormone binding site but allow the smaller insulin molecule to bind. It is interesting to note that mosquito IR homologue, which has a loop two residues larger than the

mammalian IRs, also appears to bind insulin but not IGF-1 (Graf, R., et al., 1997, *Insect Molec.Biol.* 6:151-163). Analysis of the structure indicates that the insulin/IGF-1 specificity is controlled by residues in this loop (amino acids 253-272 in IGF-1R; amino acids 260-283 in IR)

5 As chimeras only address residues which differ between the two
receptors a more precise analysis of the site can be obtained from single site
mutants. In particular, from an alanine-replacement study, four regions of L1
important for insulin binding were identified (Williams, P. F., et al., 1995, *J.*
Biol. Chem. 270:3012-3016). The first three are at similar positions on
10 successive turns of the b-helix and the fourth lies on the conserved bulge on
the large b-sheet (Figure 12). Thus there is a footprint for insulin binding to
the L1 domain which lies on the first half of large b-sheet facing into the
central space. Residues further along the sheet which are conserved in IGF-
1R and could also be important. The conservative substitution of leucine for
15 methionine at residue 119 of IR (113 of IGF-1R) causes a mild form of
leprechaunism [Hone, J. et al., 1994, *J. Med. Genet.* 31, 715-716]. This
residue is buried and the mutation could perturb neighbouring residues to
affect insulin binding.

 The axis of the L2 domain is perpendicular to that of the L1 domain
20 and N-terminal end of its β -helix is presented to the hormone-binding site.
On this face of the L2 domain the only mutation studied so far is the
naturally occurring IR mutant, S323L, which gives rise to Rabson-Mendehall
syndrome and severe insulin resistance (Roach, P., 1994, *Diabetes* 43:1096-
1102). As this mutant only affects insulin binding and not cell-surface
25 expression, residue 323 of IR (residue 313 of IGF-1R) is probably at or near
the binding site. Structurally this residue lies in the middle of a region
(residues 309-318 of IGF-1R) which is conserved in both IR and IGF-1R and
the surrounding region, 332-345 (of IGF-1R), is also quite well conserved in
the these receptors (Figure 9a). Therefore this region is quite likely to form
30 part of the hormone-binding site but would not have been detected by
chimeras. It is interesting to note that in this region IRR is not as well
conserved as the other two receptors (Shier, P. & Watt, V.M., 1989,
J.Biol.Chem. 264:4605-14608).

 The distance from this putative hormone-binding region on L2 to that
35 found on L1 is about 30 Å (Figure 8). Thus L1 and L2 appear too far apart to
bind IGF-1 or insulin. However, in the crystal structure there is a deep cleft

between part of the cys-rich domain (residue 262) and L2 (residue 305) and this cleft is occupied by a loop from a neighbouring molecule. Thus it seems probable that the position of the L2 domain in the receptor structure or the hormone-receptor complex adopts a different position with respect to the cys-rich domain than that found in the crystal. The movement required to bring L2 sufficiently close to L1 is small, namely a rotation of approximately 25° about residue 298.

A number of IR mutants have been identified which constitutively activate the receptor and the majority of these are found in the α chain. Curiously all α chain mutants involve changes to or from proline or the deletion of an amino acid, implying that they cause local structural rearrangements. The mutation R86N is similar to wild type but R86P reduces cell-surface expression and insulin binding while constitutively activating autophosphorylation [Grønskov, K. et al., 1993, *Biochem. Biophys. Res. Commun.* 192, 905-911]. The proline mutation probably disturbs residues preceding 87 which lie in the interface between the L1 and cys-rich domains but it could also affect insulin binding. In the cys-rich domain residues 233, 281, 244 and 247 of IR are not conserved in IGF-1R (Figure 9b) yet L233P [Klinkhamer, M.P. et al., 1989, *EMBO J.* 8, 2503-2507], deletion of N281 [Debois-Mouthon, C. et al., 1996, *J. Clin. Endocrinol. Metab.* 81, 719-727] or the triple mutant P243R, P244R and H247D [Rafaeloff, R. et al., 1989, *J. Biol. Chem.* 264, 15900-15904] cause constitutive kinase activation. Due to their locations each of these three mutants appears likely to compromise the folding of a β -finger domain and, in turn, the structural integrity of the rod-like cys-rich domain. The structural ramifications of these mutations could be significant for the whole receptor ectodomain as disturbing the L1/cys-rich interface or distorting the rod-like domain could affect the relative position of L1 and the cys-rich domain in this context.

L1 has been further implicated as deletion of K121 on the opposite side of L1 from the cys-rich domain was also found to cause autophosphorylation [Jospe, N. et al., 1994, *J. Clin. Endocrinol. Metab.* 79, 1294-1302]. By contrast this mutation does not affect insulin binding. Thus a possible mechanism emerges for insulin binding and signal transduction. When insulin binds between L1 and L2 it modifies the relative position of L1 and the cys-rich domain in the receptor, perhaps by hinge motion between L2 and the cys-rich domain like that suggested above, and the structural

rearrangement is transmitted across the plasma membrane. In the absence of insulin the same signal can be initiated by mutations in the cys-rich region or at the L1/cys-rich interface but at the expense on insulin binding. The signal can also be initiated more directly by mutations on the opposite side of L1
 5 which affect the interaction of L1 with other parts of the ectodomain, possibly the other half of the receptor dimer.

Ligand Studies

Although there is no structural information about an IGF-1/IGF-1R complex a number of studies have probed the nature of this interaction.
 10 Results from cross-linking experiments with IGF-1 and insulin and their cognate receptors are consistent with the hormone binding site proposed above. For example B29 of insulin can be cross-linked to the cys-rich region (residues 205-316 (Yip, C. C., et al., 1988, Biochim. Biophys. Res. Commun. 157:321-329) or the L1 domain (Wedekind, F., et al., 1989, Biol. Chem Hoppe-
 15 Seyler, 370:251-258). However these two regions are reasonably well separated and those studies may indicate that B29 is mobile. Other studies unfortunately do not map the site any more precisely.

Analogues and site-directed mutants of IGF-1 and -2 have been more fruitful. Relative to insulin IGF-1 and -2 contain two extra regions, the C
 20 region between B and A and a D peptide at the C-terminus. For IGF-1 replacement of the C region by a four Gly linker reduced affinity for IGF-1R by a factor of 40 but increased affinity for IR 5-fold (Bayne, M.L., et al., 1988, J. Biol.Chem. 264:11004-11008). Changes in affinity are consistent with the deletion in IGF-1 complementing differences in the cys-rich regions of IGF-
 25 1R and IR noted above. Mutation of residues either side of the C region (residue 24 for IGF-1 [Cascieri, M.A., et al., 1988, Biochemistry 27:3229-3233], residues 27,43 for IGF-2, [Sakano, K., et al., 1991, J. Biol. Chem. 266:20626-20635]) also have deleterious effects on the affinity of the hormone for IGF-1R as has truncation of the nearby D peptide in IGF-2 (Roth,
 30 B.V., et al., 1991, Biochem. Biophys. Res. Commun. 181:907-914). Insulin has been extensively mutated. Binding studies [summarised in Kristensen, C. et al., 1997, J. Biol. Chem. 272, 12978-12983] indicate that insulin may bind its receptor via a hydrophobic patch (residues A2, A3, A19, B8, B11, B12, B15 and possibly B23 & B24). However this patch is normally buried
 35 and requires the removal of the B chain's C-terminus from the observed position. Assuming IGF-1, -2 and insulin bind their receptors in the same

orientation, these data suggest an approximate orientation for the hormone when bound to the receptor.

One notable feature of IGF-1 and -2 is the large number of charged residues and their uneven distribution over the surface. Basic residues are predominantly found in the C region and, in solution, this region is not well ordered in either IGF-1 or -2 (Sato, A., et al., 1993, *Int J Peptide Protein Res.* 41:433-440; Torres, A. M., et al., 1995, *J. Mol. Biol.* 248:385-401). In contrast the binding site of the receptor has a sizable patch of acidic residues in the corner where the cys-rich domain departs from L1. Other acidic residues which are specific to this receptor are found along the inside face of the cys-rich domain and the loop (residues 255-263) extending from module 6. Thus it is possible that electrostatics play an important part in IGF-1 binding with the C region binding to the acidic patch of the cys-rich region near L1 and the acidic patch on the other side of the hormone directed towards a small patch of basic residues (residues 307-310) on the N-terminal end of L2.

Although the structure of this fragment gives significant information about the nature of the hormone binding site, residues outside this region have also been shown to affect binding of ligand. A number of studies have implicated residues 704-715 of IR (Mynarcik, D. C et al., 1996, *J. Biol. Chem.* 271, 2439-2442; Kurose, T., et al., 1994, *J. Biol. Chem.* 269:29190-29197). These residues could contact insulin on one of the sides left open in the current structure. Using insulin labelled at the B1 residue, Fabry, M., et al., (1992, *J. Biol. Chem.* 267:8950-8956) cross linked insulin to the fragment 390-488, part of which is not near the site as described. The explanation for this could be either 488 reaches back to the hormone binding site, or this region could contact another hormone bound to the other half of the receptor. Further structural information is needed to establish how these other regions contact the hormone and to elucidate how binding of the hormone is communicated to the kinase inside the cell.

The structure of the L1-cys-rich-L2 domains of IGF-1R presented here represents the first structural information for the extracellular portion of a member of the insulin receptor family. The L domains display a novel fold which is common to the EGF receptor family and the modular architecture of the cys-rich domain implies that smaller building blocks should be used to describe the composition of cysteine-rich domains. This fragment contains the major specificity determinants of receptors of this class for their ligands.

It has an elongated structure with a space in the middle which could accommodate the ligand. The three sides of this site correspond to regions which have been implicated in hormone binding. Although other sites are present in the receptor ectodomain which interact with the ligand this structure gives us an initial view of how the insulin, IGF-1 and -2 might interact with their cell surface receptors to control their metabolic and mitogenic effects

Such information will provide valuable insight into the structure of the corresponding domains of the IR and insulin receptor-related receptor as well as members of the related EGFR family (Bajaj, M., et al., 1987, Biochim Biophys Acta 916:220-226; Ward, C. W. et al., 1995, Proteins: Struct Funct Genet 22:141-153).

EXAMPLE 4

Prediction of 3D Structure of the Corresponding Domains of IRR and IR Based on Structure of IGF-1R Frgament.

The sequence identities between the different members of the insulin receptor family are sufficient to allow accurate sequence alignments to facilitate 3D structure predictions by homology modelling. The alignments of the ectodomains of human IGF-1R, IR, and IRR are shown in Figure 13.

EXAMPLE 5

Prediction of 3D Structure of EGFR and its Family Members ERB2, ERB3 and ERB4.

The sequence identities between the different members of the EGFR receptor family and the insulin receptor family are sufficient to allow accurate sequence alignments to facilitate 3D structure predictions by homology modelling. The alignments of the ectodomains of human EGFR, ERB2, ERB3 and ERB4 are shown in Figure 14. The ectodomains of the EGFR family members are composed of four domains : L1 domain, cys-rich domain, L2 domain and a second cys-rich domain all of which can be modelled from the structure of the IGF-1R fragment residues 1-462.

The sequence alignment analysis and characterization of the repeat modules in the cys-rich region of IGF-1R and the homologous regions of the

IR, IRR and the first and second cys-rich regions of EGFR, ErbB2, ErbB3 and ErbB4 are shown in Figure 15. A representative of each subtype of cys repeat is found in the IGF-1R fragment 1-462 and is used to model each of these modules in the other receptors. Note the nature and order of modules in the second cys-rich repeat of the EGFR family is different to that seen in the first cys-rich region.

EXAMPLE 6

Single-Molecule Imaging of Human Insulin Receptor Ectodomain and its Fab Complexes

10 Cloning and expression of hIR -11 ectodomain protein

A full length clone of the human IR exon -11 form (hIR -11) was prepared by exchanging an Aat II fragment, nucleotides 1195 to 2987, of the exon +11 clone (plasmid pET; Ellis et al., 1986; gift from Dr W. J. Rutter, UCSF) of hIR (Ebina et al., 1985, *Cell* 40, 747-758) with the equivalent Aat II fragment from a plasmid (pHIR/P12-1, ATCC 57493) encoding part of the extracellular domain and the entire cytoplasmic domain of hIR -11 (Ullrich et al., 1985, *Nature* 313, 756-761). The ectodomain fragment of hIR -11 (2901 bp, coding for the 27 residue signal sequence and residues His1-Asn914) was produced by SalI and SspI digestion and inserted into the mammalian expression vector pEE6.HCMV-GS (Celltech Limited, Slough, Berkshire, UK) into which a stop codon linker had been inserted, as described previously (Cosgrove et al., 1995, *Protein Expression and Purification* 6, 789-798) for the hIR exon +11 ectodomain.

The resulting recombinant plasmid pHIR II (2 µg) was transfected into glycosylation deficient Chinese hamster ovary (Lec 8) cells (Stanley, 1989, *Molec. Cellul. Biol.* 9, 377-383) with Lipofectin (Gibco-BRL). After transfection, the cells were maintained in glutamine-free medium GMEM (ICN Biomedicals, Australia) as described previously (Bebbington & Hentschel, 1987, In *DNA Cloning* (Glover, D., ed.), Vol III, Academic Press, San Diego; Cosgrove et al., 1995, *Protein Expression and Purification* 6, 789-798). Expressing cell lines were selected for growth in GMEM with 25 µM methionine sulfoximine (MSX, Sigma). Transfectants were screened for protein expression using sandwich ELISA with anti-IR monoclonal antibodies 83-7 and 83-14. Metabolic labelling of cells, immunoprecipitations, insulin binding assays and Scatchard analyses were performed as described

previously for the exon +11 form of hIR ectodomain (Cosgrove et al., 1995, , *Protein Expression and Purification* 6, 789-798).

hIR -11 ectodomain production and purification

The selected clone (inoculum of 1.28×10^8 cells) was grown in a
 5 spinner flask packed with 10 g of Fibra-cel disc carriers (Sterilin, U.K.) in 500 ml of GMEM medium containing 10% fetal calf serum (FCS) and 25 μ M MSX. Selection pressure was maintained for the duration of the culture.

Ectodomain was recovered from harvested media by affinity
 chromatography on immobilized insulin and further purified by gel filtration
 10 chromatography on Superdex S200 (Pharmacia; 1 x 40 cm) in Tris-buffered saline containing 0.02% sodium azide (TBSA) as described previously (Cosgrove et al., 1995, *Protein Expression and Purification* 6, 789-798). Solutions of purified hIR -11 ectodomain were stored at 4° C prior to use.

Production of Fab fragments and their complexes with ectodomain

15 Purification of Mabs 83-7, 83-14 and 18-44 from ascites fluid by affinity chromatography using Protein A-Sepharose, and the production of Fabs, were based on the methodologies described in Coligan et al., 1993, Current Protocols in Immunology, Vol 1, pp 2.7.1-2.8.9, Greene Publishing Associates & Wiley - Interscience, John Wiley and Sons. Fab was produced
 20 from monoclonal antibody by mercuripapain digestion for 1-4 h, followed by gel filtration on Superdex S200. Products were monitored by reducing and non-reducing SDS-PAGE. For 83-7 Mab, an IgG Type 1 monoclonal antibody, the bivalent (Fab)₂' isolated by this method was reduced to monovalent Fab 83-7 by mild reduction with mM L-cysteine.HCl in 100 mM Tris pH 8.0
 25 (Coligan et al., 1993, Current Protocols in Immunology, Vol 1, pp 2.7.1-2.8.9, Greene Publishing Associates & Wiley - Interscience, John Wiley and Sons).

Complexes of Fab with hIR -11 ectodomain were produced by mixing
 ~ 2.5 to 3.5 molar excess of Fab with hIR -11 ectodomain at ambient
 temperature in TBSA at pH 8.0. After 1-3 h, the complex was separated from
 30 unbound Fab by gel filtration over a Superdex S200 column in the same buffer.

Electron microscopy

Uncomplexed hIR -11 ectodomain and the Fab complexes described
 above were diluted in phosphate-buffered saline (PBS) to concentrations of
 35 the order of 0.01-0.03 mg/ml. Prior to dilution, 10% glutaraldehyde (Fluka) was added to the PBS to achieve a final concentration of 1% glutaraldehyde.

Droplets of ~ 3ml of this solution were applied to thin carbon film on 700-mesh gold grids after glow-discharging in nitrogen for 30 s. After 1 min. the excess protein solution was drawn off and followed by application and withdrawal of 4-5 droplets of negative stain [2% uranyl acetate (Agar), 2% uranyl formate (K and K), 2% potassium phosphotungstate (Probing and Structure) adjusted to pH 6.0 with KOH, or 2% methylamine tungstate (Agar) adjusted to pH 6.8 with NH₄OH]. In the case of both uranyl acetate and uranyl formate staining, an intermediate wash with 2 or 3 droplets of PBS was included prior to application of the stain. The grids were air-dried and then examined at 60kV accelerating voltage in a JEOL 100B transmission electron microscope at a magnification of 100,000x. It was found that there was a typical thickness of negative stain in which Fabs were most easily seen, hence areas for photography had to be chosen from particular zones of the grid. Electron micrographs were recorded on Kodak SO-163 film and developed in undiluted Kodak D19 developer. The electron-optical magnification was calibrated under identical imaging conditions by recording single-molecule images of the antigen-antibody complex of influenza virus neuraminidase heads and NC10 MFab (Tulloch et al., 1986, *J. Mol. Biol.* 190, 215-225; Malby et al., 1994, *Structure*, 2, 733-746).

20 Image processing

Electron micrographs showing particles in a limited number of identifiable projections were chosen for digitisation. Micrographs were digitised on a Perkin-Elmer model 1010 GMS PDS flatbed scanning microdensitometer with a scanning aperture (square) size of 20 mm and stepping increment of 20 mm corresponding to a distance of 0.2 nm on the specimen. Particles were selected from the digitised micrograph using the interactive windowing facility of the SPIDER image processing system (Frank et al., 1996, *J. Struct. Biol.* 116, 190-199). Particles were scaled to an optical density range of 0.0 - 2.0 and aligned by the PSPC reference-free alignment algorithm (Marco et al., 1996, *Ultramicroscopy*, 66, 5-10). Averages were then calculated over a subset of correctly aligned particles chosen interactively as being representative of a single view of the particle. The final average image presented here is derived from a library of 94 images.

Biochemical characterization of expressed hIR -11 ectodomain

35 The recombinant protein examined corresponded to the the first 914 residues of the 917 residue ectodomain of the exon -11 form of the human

insulin receptor (Ullrich et al., 1986, *Nature* 313 , 756-761). Expressed protein was shown, by SDS-PAGE and autoradiography of immunoprecipitated product from metabolically labelled cells, to exist as a homodimeric complex of ~270 - 320 kDa apparent mass, which dissociated under reducing
 5 conditions into monomeric α and β' subunits of respective apparent mass ~120 kDa and ~35 kDa (data not shown).

Purified hIR -11 ectodomain, expressed in Lec8 cells and purified by affinity chromatography on an insulin affinity column, ran as a symmetrical peak on a Superdex S200 gel filtration column (Figure 16). The protein eluted
 10 with an apparent mass of ~400 kDa, calculated from a standard curve generated by the elution positions of standard proteins (not shown). As expected for protein expressed in Lec 8 cells, whose glycosylation defect produces truncated oligosaccharides (Stanley, 1989, *Molec. Cellul. Biol.* 9, 377-383), this value is less than the apparent mass (450 - 500 kDa) reported
 15 for hIR +11 ectodomain expressed in wild-type CHO-K1 cells (Johnson et al., 1988, *Proc. Natl Acad. Sci USA* 85, 7516-7520; Cosgrove et al., 1995, *Protein Expression and Purification* 6, 789-798).

Radioassay of insulin binding to purified ectodomain gave linear Scatchard plots and Kd values of $1.5 - 1.8 \times 10^{-9}$ M, similar to the values of
 20 $2.4 - 5.0 \times 10^{-9}$ M reported for the hIR -11 ectodomain (Andersen et al., 1990, *Biochemistry* 29, 7363-7366; Markussen et al., 1991, *J. Biol. Chem.* 266, 18814-18818; Schaffer, 1994, *Eur. J. Biochem.* 221, 1127-1132) and the values of $\sim 1.0 - 5.0 \times 10^{-9}$ M reported for the hIR +11 ectodomain (Schaefer et al., 1992, *J. Biol. Chem.* 267, 23393-23402; Whittaker et al., 1994, *Molec.*
 25 *Endocrinol.* 8, 1521-1527; Cosgrove et al., 1995, *Protein Expression and Purification* 6, 789-798).

Expression of hIGF-1R ectodomain

Cloning, expression and purification of this protein used elements common to those described for hIR -11 ectodomain (Cosgrove et al., 1995,
 30 *Protein Expression and Purification* 6, 789-798) and resulted in purified product that was recognised by receptor-specific Mabs 17-69, 24-31 and 24-60 (Soos et al., 1992, *J. Biol. Chem.* 267, 12955-63) and was composed of α and β' subunits of mass similar to those of hIR ectodomain (unpublished data).

Preparation of hIR -11 ectodomain/MFab complexes

35 A complex of hIR -11 ectodomain and Fab from antibody 83-14 eluted as a symmetrical peak of 460 -500 kDa (Figure 16), as did complexes

generated from a mixture of hIR -11 ectodomain with Fab from antibody 18-44 and a mixture of hIR -11 ectodomain with Fab 83-7 (not shown). A co-complex of ectodomain with Fabs from antibodies 18-44 and 83-14 eluted at ~ 620 kDa (Figure 12), as did a co-complex with MFabs 83-14/83-7 and another with MFabs 83-7/18-44 (not shown). A complex of hIR -11
 5 ectodomain with all three MFab derivatives, 18-44, 83-7 and 83-14, eluted at an apparent mass of ~ 710 kDa (Figure 16).

Electron microscopy

Imaging of hIR -11 and hIGF-1R ectodomains

10 Single-molecule imaging of undecorated dimeric hIR -11 ectodomain was carried out under a variety of negative staining conditions, which emphasised different aspects of the structure of the molecular envelope. The least aggressive or penetrative stain was potassium phosphotungstate (KPT) , which revealed consistent globular particles with very little internal structure
 15 other than a suggestion of a division into two parallel bars. Staining with methylamine tungstate also revealed the parallel bar images, as shown in Figure 17a.

Further investigation using progressively more penetrative, but also potentially more disruptive, stains confirmed the observations above.
 20 Staining with uranyl acetate and uranyl formate showed the separation of the parallel bars most clearly (Figure 17b), but uranyl acetate showed evidence of disrupting the structure of the particles, i.e. a decrease in the consistency of the particle shape and a tendency for particles to look unravelled or denatured despite having been subjected to chemical cross-linking prior to
 25 staining. In areas of thicker stain, parallel bars predominated (Figure 17b) , whereas in more thinly stained regions, U-shaped particles could be identified, sometimes outnumbering the parallel-bar structures (Figure 18a). An averaged image of the parallel bars seen by staining hIR -11 ectodomain with uranyl formate is shown as an insert in Figure 17b.

30 In Figures 17c and 18b, images of hIGF-1R ectodomain are shown for comparison with Figure 17b and 18a, respectively, under similar staining conditions.

Imaging of hIR -11 ectodomain complexed with 83-7 MFab

This complex was particularly noteworthy for the consistency of the
 35 form of the particles, especially under the gentler staining conditions afforded by stains such as KPT and methylamine tungstate. The particles

were interpreted as having been restricted in the views they presented, after air-drying on the carbon support film, by the almost diametrically opposite binding of the two Fab arms to the antigen to form a highly elongated complex structure. Under these conditions three distinct views could be
 5 recognised as shown in Figure 19. Two views (interpreted as top-down/bottom-up) show the Fab arms displaced clockwise or anti-clockwise as extensions of the parallel plates with two-fold symmetry. The third view shows an image with the two Fab arms in line roughly through the centre of the receptor on its opposite sides, interpreted as a side projection of binding
 10 half-way up the plates (Figure 19).

Figure 20 shows a field of particles of hIR -11 ectodomain complexed with 83-7 MFab, stained with uranyl formate. The use of the more aggressive uranyl stains operating at lower pHs revealed internal structure of the molecular envelope at the expense of consistency of the particle morphology.
 15 For example, staining with uranyl acetate or uranyl formate showed that parallel bars can be seen in particles in which the Fab arms are displaced either clockwise or anticlockwise but not where the intermediate central or axial position of the two Fab arms is presented in projection. These observations show 83-7 MFab binding roughly half-way up the side-edge of
 20 each hIR -11 ectodomain plate. The epitope recognised by Mab 83-7 has been mapped to the cys-rich region, residues 191-297, by analysis of chimeric receptors (Zhang and Roth, 1991, *Proc. Natl. Acad. Sci. USA* **88**, 9858-9862).

25 **Imaging of hIR -11 ectodomain complexed with either 83-14 MFab or 18-44 MFab**

Figure 21a shows the complexes formed with Fabs from the most insulin-mimetic antibody Mab 83-14. Projections showing the Fab arms bound to and extending out from near the base of the U-shaped particles can
 30 be identified. A second field of particles (Figure 21b) shows objects composed of two parallel bars as observed for the undecorated ectodomain, with Fab arms projecting obliquely from diametrically opposite extremities. Similar but less definitive images were also seen when MFab 18-44 was bound to hIR -11 ectodomain (not shown). The epitope for Mab 83-14 is
 35 between residues 469-592 (Prigent et al., 1990) in the connecting domain. This domain contains one of the disulphide bonds (Cys524-Cys524) between

the two monomers in the IR dimer (Schaffer and Ljungqvist, 1992, *Biochem. Biophys. Res. Commun.* **189**, 650-653). The epitope for Mab 18-44 is a linear epitope, residues 765-770 (Prigent et al., 1990, *J. Biol. Chem.* **265**, 9970-9977) in the β -chain, near the end of the insert domain (O'Bryan et al., 1991, *Mol. Cell. Biol.* **11**, 5016-5031). The insert domain contains the second disulphide bond connecting the two monomers in the IR dimer (Sparrow et al., 1997, *J. Biol. Chem.*, **272**, 29460-29467).

Imaging of hIR -11 ectodomain co-complexed with two different MFabs per monomer

The double complex of hIR -11 ectodomain with MFabs 83-7 and 18-44 was stained with 2% KPT at pH 6.0, and revealed the molecular envelopes shown in Figure 22. The particle appears complex in shape and can assume a number of different orientations on the carbon support film, giving rise to a number of different projections in the micrograph. The predominant view is of an asymmetric X-shape (some examples circled). It shows the 83-7 MFab arms bound at opposite ends of the parallel bars with the two 18-44 MFabs appearing as shorter projections extending out from either side of each ectodomain.

Images of the double complex of hIR -11 ectodomain with 83-7 and 83-14 MFabs gave X-shaped images similar to those seen with the 83-7/18-44 double complex (not shown). In contrast the double complex of hIR -11 ectodomain with 18-44 and 83-14 MFabs did not present the characteristic asymmetric X-shapes described above (images not shown). Instead, the molecular envelope appeared to be elongated in many views, with only an occasional X-shaped projection. While a detailed interpretation of these images would be premature, it is clear that MFabs 18-44 and 83-14, two of the more potent insulin mimetic antibodies (Prigent et al., 1990, *J. Biol. Chem.* **265**, 9970-9977), can bind simultaneously to the receptor.

Imaging of hIR -11 ectodomain co-complexed with three different MFabs per monomer

Figure 23 shows a field of particles from a micrograph of hIR -11 ectodomain complexed simultaneously with MFabs 83-7, 83-14 and 18-44. In the thicker stain regions the molecular envelope is X-shaped, and looks very similar to that of the double complexes of hIR -11 ectodomain with either 83-7 and 18-44 or 83-7 and 83-14. However, in the more thinly stained regions, particles of greater complexity are visible and it is possible occasionally to

identify that there are in fact more than four MFabs bound to the ectodomain dimer.

The single-molecule imaging of hIR -11 ectodomain presented here suggests a molecular envelope for this dimeric species significantly different from that of any previously published study. However, an unequivocal determination of the molecular envelope even from the present study is not entirely straightforward. A major complicating factor here has been the relative fragility of the expressed ectodomain when exposed to the rigors of electron microscope preparation by negative staining. For example, staining with potassium phosphotungstate (KPT, pH 6.0-7.0) frequently suggested a denaturation of the dimeric molecules, but when appropriate conditions were satisfied, good seemingly interpretable molecular envelope images were achieved; staining with methylamine tungstate (pH ~7.0) supported the best KPT molecular envelope images, but had the suggestion of a swelling of the molecular structure at neutral pH; and the acid-pH stains of uranyl acetate (pH ~4.2) and uranyl formate (pH~3.0), with their ability to penetrate the ectodomain structure, appeared to illuminate not so much the molecular envelope as the zones of high projected protein density within the dimer.

An amalgam of impressions from these various staining regimens has led to the following interpretation of single-molecule images of these undecorated, or naked, dimers: the predominant dimeric molecular image encountered here has been that of 'parallel bars' of projected protein density. This view is so predominant, indeed, that it suggests there is either a single preferred orientation of the molecules on the glow-discharged carbon support film, or that this impression of parallel bars of density may represent a mixture of superficially similar structure projections, with the subtleties of these different projections being masked by the relatively coarse resolution of this single-molecule direct imaging. The impression of parallel bars of projected protein density is particularly predominant in regions of thicker negative stain. A second view of the molecular envelope, appreciably less well represented in regions of thicker stain but predominant in regions of thin staining, is that of 'open' U's, or V's. These two views of hIR -11 ectodomain were supported by the single-molecule imaging of hIGF-1R ectodomain under comparable conditions of negative staining.

If the assumption is made that these two recognisable projected views, that of parallel bars and of open U's/V's, are different views of the

same dimeric molecule, an assumption strongly supported by the MFab complex imaging, a coarse model of the molecular envelope can be rationalized as in the schematic Figure 24. The model structure is roughly that of a cube, composed of two almost-parallel plates of high protein
 5 density, separated by a deep cleft of low protein main-chain and side-chain density able to be penetrated by stain, and connected by intermediate stain-excluding density near what is assumed here to be their base (that is, nearest the membrane-anchoring region). The width of the low-density cleft appears to be of the order of 30-35Å, sufficient to accommodate the binding
 10 of the insulin molecule of diameter ca. 30Å, although we have no electron microscopical evidence to support insulin-binding in this cleft at this stage.

It has been established through imaging of bound 83-7 MFab that there is a dimeric two-fold axis normal to the membrane surface between these plates of density. Occasionally, dimer images display a relative
 15 displacement of the bars of density, interpreted here as a limited capacity for a shearing of the interconnecting zone between the two plates along their horizontal axis parallel to the membrane; other images show bars skewed from parallel, implying a limited capacity for the plates to rotate independently around the two-fold axis, again via this interconnecting zone.
 20 These two observations each suggest a relatively flexible connectivity between the dimer plates in the membrane-proximal region of intermediate protein density, which could possibly contribute to the transmembrane signalling process.

The approximate overall measured dimensions of the ectodomain dimer depicted in Figure 24 are 110 x 90 x 120Å, calibrated against the dimensions of imaged influenza neuraminidase heads, known from the solved X-ray structure (Varghese et al., 1983, *Nature* 303, 35-40). It can be noted that there is a compatibility here between the molecular weights and molecular dimensions of these two molecular species: the compact
 30 tetrameric influenza neuraminidase heads of Mr ~200 kDa occupy a volume almost 100 x 100 x 60 Å; the more open dimeric insulin receptor ectodomains of similar Mr ~240 kDa imaged here occupy a volume approximately 110 x 90 x 120 Å . roughly twice that of the neuraminidase heads, accommodating the slightly higher molecular weight and substantial central low-density cleft.

35 The low-resolution roughly cubic compact structure proposed here differs substantially from the T-shaped model proposed by Christiansen et al.

(1991, *Proc. Natl. Acad. Sci. U. S. A.* **88**, 249-252) and Tranum-Jensen et al., (1994, *J. Membrane Biol.* **140**, 215-223) for the whole receptor and the elongated model proposed by Schaefer et al. (1992, *J. Biol. Chem.* **267**, 23393-23402) for soluble ectodomain. Significantly, those previous studies did not
 5 provide any convincing independent electron microscopical evidence that their imaged objects were in fact insulin receptor.

In the present study, the identity of the imaged molecules as hIR -11 ectodomain has been confirmed by imaging complexes of the dimer with Fabs of the three well-established conformational Mabs against native hIR,
 10 83-7, 83-14 and 18-44 (Soos et al., 1986, *Biochem. J.* **235**, 199-208; 1989, *Proc. Natl Acad. Sci. USA* **86**, 5217-5221), bound singly and in combination. In all these instances, virtually every particle in the field of view exhibited MFab decoration through binding to conformational epitopes, establishing not only the identity of the imaged particles but also the conformational integrity of
 15 the expressed ectodomains. Furthermore, the cleanliness and uniformity of these hIR -11 ectodomain preparations, both naked and decorated, visualised here by electron microscopy demonstrate their high suitability for X-ray crystallization trials.

The known flexibility of the Fab arms exacerbates image-to-image variability beyond the limited extent already described for the undecorated dimeric ectodomains, complicating any precise interpretation of these antigen-antibody complexes. Such molecular flexibility also renders largely impractical any single-molecule computer image averaging to facilitate image interpretation, progressively more so with the higher order antigen-antibody
 25 complexes studied here.

The most readily interpretable of these images, showing least image-to-image variability, are those of 83-7 MFab bound to dimers where, fortuitously, the antigen-antibody complex is constrained in its degrees of rotational freedom on the carbon support film. Many projected images show
 30 the two Fab arms in line roughly through the centre of the antigen on its opposite sides (Figure 19, arrowed examples), interpreted as a side projection of binding half-way up the plates from their membrane-proximal base. Other sub-sets of images (Figure 19, circled examples) show the two Fab arms still parallel but displaced clockwise or anticlockwise with 2-fold
 35 symmetry, each Fab approximating an extension of one of the parallel bars of antigen density, interpreted here as representing top or bottom projections

along the 2-fold axis. The third projection, along the axis of the Fab arms, could not be sampled here because of the constraining geometry of this molecular complex. These observations suggest binding of 83-7 MFab roughly half-way up the side-edge of the hIR -11 ectodomain plate. This then allows an initial attempt at spatially mapping the 83-7 MFab epitope, which has been sequence-mapped to residues 191-297 in the cys-rich region of the insulin receptor (Zhang and Roth, 1991, *Proc. Natl. Acad. Sci. USA* **88**, 9858-9862). The spatial separation and relative orientations of the two binding epitopes of Mab 83-7 on the hIR -11 ectodomain dimer as indicated here appear inconsistent with the proposal that Mab 83-7 could bind intramolecularly to hIR (O'Brien et al., 1987, *Biochem J.* **6**, 4003-4010).

Decoration of the ectodomain dimer with 83-7 MFab established that the two plates of high protein-density are arranged with 2-fold symmetry. Decoration with either 83-14 or 18-44 MFab, on the other hand, allowed sampling of the third projection of the ectodomain dimer precluded by 83-7 MFab binding. Significantly, this third view established unequivocally the U-shaped projection of the hIR -11 ectodomain dimer, something which was only able to be assumed with the undecorated ectodomain images. Further, this projection has allowed a rough spatial mapping close to the base of the U-shaped dimer for the epitopes recognised by 83-14 MFab (residues 469-592, connecting domain) and 18-44 MFab (residues 765-770, b-chain insert domain; exon 11 plus numbering, Prigent et al., 1990, *J. Biol. Chem.* **265**, 9970-9977).

Inherent in the model structure presented in Figure 20 is the implication that, with the two-fold axis aligned normal to the membrane surface, the mouth of the low-density cleft where insulin binding may occur would lie most distant from the transmembrane anchor, whilst the zone of intermediate density connecting the two high-density plates would be in close proximity to the membrane. It follows, in this model, that the L1/cys-rich/L2 domains (Bajaj et al., 1997, *Biochim. Biophys. Acta* **916**, 220-226; Ward et al., 1995, *Proteins: Struct., Funct., Genet.* **22**, 141-153), which comprise much of the insulin-binding region (see Mynarcik et al., 1997, *J. Biol. Chem.* **272**, 2077-2081), most probably lie in the membrane-distal upper halves of the two plates, whilst the membrane-proximal lower halves contain the connecting domains, the fibronectin-type domains, the insert domains and the interchain disulphide bonds (Schaffer and Ljungqvist, 1992, *Biochem.*

Biophys. Res. Commun. 189, 650-653; Sparrow et al., 1997, *J. Biol. Chem.*, 272, 29460-29467). Such a disposition of domains is supported by the images seen with the single MFab decoration, the 83-7 MFab epitope in the cys-rich region being spatially mapped roughly half-way up the side-edge of the
 5 ectodomain plates, and the 83-14 and 18-44 MFab epitopes (connecting domain and β -chain insert domain, respectively) being mapped near the base of the plates. Our preference is for a single a-b ϵ monomer to occupy a single plate, although the possibility of a single monomer straddling the two plates of protein density cannot be discounted.

10 The more complex images involving co-binding of two, and even more so of all three, MFabs to each monomer of the ectodomain dimer (Figures 22 and 23) are not easily interpretable with respect to relative domain arrangements within the monomer at present, not least of all because of the difficulty of finding conditions of negative staining that will
 15 simultaneously maintain the integrity of the Fab binding while highlighting recognisable and reproducible details of the internal structure of the dimeric IR ectodomain.

The data presented here demonstrate the ability of single-molecule imaging to give an initial insight into the topology of multidomain structures
 20 such as the ectodomain of hIR, and the value of combining this technique with that of either single or multiple monoclonal Fab attachment per monomer as a potential means of epitope (and domain) mapping of the structure. By imaging Fab complexes of other members of the family (such as hIGF-1R ectodomain) and combining available sequence-mapped epitope
 25 information with that presented here, a more comprehensive understanding of domain arrangements within the IR family ectodomains should be forthcoming.

It will be appreciated by persons skilled in the art that numerous variations and/or modifications may be made to the invention as shown in
 30 the specific embodiments without departing from the spirit or scope of the invention as broadly described. The present embodiments are, therefore, to be considered in all respects as illustrative and not restrictive

Dated this twenty-fourth day of March 1998

COMMONWEALTH SCIENTIFIC
AND INDUSTRIAL RESEARCH
ORGANISATION

Patent Attorneys for the Applicant:

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Figure 1

| | | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 1 | CB | GLU | 1 | 55.907 | 11.926 | 66.300 | 1.00 | 59.11 | AAAA | C |
| ATOM | 2 | CG | GLU | 1 | 56.138 | 11.019 | 65.162 | 1.00 | 78.17 | AAAA | C |
| ATOM | 3 | CD | GLU | 1 | 57.382 | 11.319 | 64.321 | 1.00 | 85.10 | AAAA | C |
| ATOM | 4 | OE1 | GLU | 1 | 58.404 | 10.754 | 64.796 | 1.00 | 86.18 | AAAA | O |
| ATOM | 5 | OE2 | GLU | 1 | 57.424 | 12.013 | 63.270 | 1.00 | 78.70 | AAAA | O |
| ATOM | 6 | C | GLU | 1 | 53.508 | 12.557 | 66.350 | 1.00 | 48.46 | AAAA | C |
| ATOM | 7 | O | GLU | 1 | 52.685 | 11.863 | 65.784 | 1.00 | 51.27 | AAAA | O |
| ATOM | 10 | H | GLU | 1 | 54.256 | 10.339 | 67.159 | 1.00 | 61.64 | AAAA | H |
| ATOM | 12 | CA | GLU | 1 | 54.602 | 11.778 | 67.081 | 1.00 | 54.77 | AAAA | C |
| ATOM | 13 | H | ILE | 2 | 53.608 | 13.860 | 66.375 | 1.00 | 37.66 | AAAA | H |
| ATOM | 15 | CA | ILE | 2 | 52.768 | 14.699 | 65.604 | 1.00 | 40.87 | AAAA | C |
| ATOM | 16 | CB | ILE | 2 | 52.925 | 16.122 | 66.160 | 1.00 | 41.97 | AAAA | C |
| ATOM | 17 | CG2 | ILE | 2 | 52.036 | 17.122 | 65.484 | 1.00 | 38.50 | AAAA | C |
| ATOM | 18 | CG1 | ILE | 2 | 52.560 | 16.006 | 67.663 | 1.00 | 46.58 | AAAA | C |
| ATOM | 19 | CD1 | ILE | 2 | 53.150 | 17.176 | 68.498 | 1.00 | 32.29 | AAAA | C |
| ATOM | 20 | C | ILE | 2 | 53.122 | 14.711 | 64.139 | 1.00 | 46.47 | AAAA | C |
| ATOM | 21 | O | ILE | 2 | 54.258 | 15.029 | 63.852 | 1.00 | 51.66 | AAAA | O |
| ATOM | 22 | H | CYS | 3 | 52.235 | 14.409 | 63.196 | 1.00 | 49.61 | AAAA | H |
| ATOM | 24 | CA | CYS | 3 | 52.435 | 14.677 | 61.773 | 1.00 | 38.93 | AAAA | C |
| ATOM | 25 | C | CYS | 3 | 51.429 | 15.708 | 61.302 | 1.00 | 42.06 | AAAA | C |
| ATOM | 26 | O | CYS | 3 | 50.290 | 15.521 | 61.690 | 1.00 | 42.37 | AAAA | O |
| ATOM | 27 | CB | CYS | 3 | 52.159 | 13.415 | 60.999 | 1.00 | 35.66 | AAAA | C |
| ATOM | 28 | SG | CYS | 3 | 53.019 | 12.004 | 61.674 | 1.00 | 36.98 | AAAA | S |
| ATOM | 29 | H | GLY | 4 | 51.851 | 16.709 | 60.580 | 1.00 | 42.39 | AAAA | H |
| ATOM | 31 | CA | GLY | 4 | 50.973 | 17.718 | 60.003 | 1.00 | 47.71 | AAAA | C |
| ATOM | 32 | C | GLY | 4 | 51.703 | 18.407 | 58.869 | 1.00 | 48.23 | AAAA | C |
| ATOM | 33 | O | GLY | 4 | 52.916 | 18.345 | 58.884 | 1.00 | 55.36 | AAAA | O |
| ATOM | 34 | H | PRO | 5 | 51.056 | 19.212 | 58.048 | 1.00 | 49.63 | AAAA | H |
| ATOM | 35 | CD | PRO | 5 | 51.637 | 19.947 | 56.860 | 1.00 | 45.28 | AAAA | C |
| ATOM | 36 | CA | PRO | 5 | 49.605 | 19.341 | 58.083 | 1.00 | 41.57 | AAAA | C |
| ATOM | 37 | CB | PRO | 5 | 49.397 | 20.703 | 57.474 | 1.00 | 44.30 | AAAA | C |
| ATOM | 38 | CG | PRO | 5 | 50.632 | 21.036 | 56.693 | 1.00 | 46.43 | AAAA | C |
| ATOM | 39 | C | PRO | 5 | 48.932 | 19.217 | 57.354 | 1.00 | 36.40 | AAAA | C |
| ATOM | 40 | O | PRO | 5 | 49.403 | 17.094 | 57.396 | 1.00 | 43.35 | AAAA | O |
| ATOM | 41 | H | GLY | 6 | 47.787 | 18.439 | 56.795 | 1.00 | 39.15 | AAAA | H |
| ATOM | 43 | CA | GLY | 6 | 46.896 | 17.336 | 56.350 | 1.00 | 39.24 | AAAA | C |
| ATOM | 44 | C | GLY | 6 | 47.710 | 16.365 | 55.523 | 1.00 | 33.68 | AAAA | C |
| ATOM | 45 | O | GLY | 6 | 48.510 | 16.863 | 54.753 | 1.00 | 36.00 | AAAA | O |
| ATOM | 46 | H | ILE | 7 | 47.586 | 15.111 | 55.788 | 1.00 | 35.70 | AAAA | H |
| ATOM | 48 | CA | ILE | 7 | 48.307 | 14.053 | 55.141 | 1.00 | 37.65 | AAAA | C |
| ATOM | 49 | CB | ILE | 7 | 48.556 | 12.797 | 55.933 | 1.00 | 36.31 | AAAA | C |
| ATOM | 50 | CG2 | ILE | 7 | 49.043 | 11.700 | 54.988 | 1.00 | 34.67 | AAAA | C |
| ATOM | 51 | CG1 | ILE | 7 | 49.561 | 12.857 | 57.067 | 1.00 | 39.34 | AAAA | C |
| ATOM | 52 | CD1 | ILE | 7 | 49.678 | 14.249 | 57.669 | 1.00 | 40.22 | AAAA | C |
| ATOM | 53 | C | ILE | 7 | 47.338 | 13.762 | 53.977 | 1.00 | 45.00 | AAAA | C |
| ATOM | 54 | O | ILE | 7 | 46.150 | 13.643 | 54.195 | 1.00 | 51.52 | AAAA | O |
| ATOM | 55 | H | ASP | 8 | 47.767 | 13.631 | 52.751 | 1.00 | 45.60 | AAAA | H |
| ATOM | 57 | CA | ASP | 8 | 46.938 | 13.293 | 51.631 | 1.00 | 44.05 | AAAA | C |
| ATOM | 58 | CB | ASP | 8 | 47.003 | 14.469 | 50.651 | 1.00 | 44.21 | AAAA | C |
| ATOM | 59 | CG | ASP | 8 | 45.909 | 14.379 | 49.600 | 1.00 | 43.49 | AAAA | C |
| ATOM | 60 | OD1 | ASP | 8 | 45.660 | 13.262 | 49.096 | 1.00 | 51.77 | AAAA | O |
| ATOM | 61 | OD2 | ASP | 8 | 45.253 | 15.374 | 49.251 | 1.00 | 46.94 | AAAA | O |
| ATOM | 62 | C | ASP | 8 | 47.428 | 12.000 | 50.992 | 1.00 | 42.16 | AAAA | C |
| ATOM | 63 | O | ASP | 8 | 48.423 | 12.143 | 50.330 | 1.00 | 48.50 | AAAA | O |
| ATOM | 64 | H | ILE | 9 | 47.096 | 10.817 | 51.321 | 1.00 | 42.76 | AAAA | H |
| ATOM | 66 | CA | ILE | 9 | 47.441 | 9.505 | 50.939 | 1.00 | 44.05 | AAAA | C |
| ATOM | 67 | CB | ILE | 9 | 47.212 | 8.483 | 52.077 | 1.00 | 40.82 | AAAA | C |
| ATOM | 68 | CG2 | ILE | 9 | 47.669 | 7.085 | 51.653 | 1.00 | 36.35 | AAAA | C |
| ATOM | 69 | CG1 | ILE | 9 | 47.888 | 8.917 | 53.364 | 1.00 | 41.17 | AAAA | C |
| ATOM | 70 | CD1 | ILE | 9 | 49.376 | 9.947 | 53.286 | 1.00 | 43.78 | AAAA | C |
| ATOM | 71 | C | ILE | 9 | 46.530 | 9.137 | 49.794 | 1.00 | 51.49 | AAAA | C |
| ATOM | 72 | O | ILE | 9 | 45.338 | 9.420 | 49.832 | 1.00 | 63.05 | AAAA | O |
| ATOM | 73 | H | ARG | 10 | 47.004 | 9.417 | 48.812 | 1.00 | 54.87 | AAAA | H |
| ATOM | 75 | CA | ARG | 10 | 46.283 | 8.089 | 47.600 | 1.00 | 54.17 | AAAA | C |
| ATOM | 76 | CB | ARG | 10 | 45.703 | 9.358 | 47.023 | 1.00 | 48.54 | AAAA | C |
| ATOM | 77 | CG | ARG | 10 | 46.361 | 10.169 | 45.952 | 1.00 | 46.55 | AAAA | C |
| ATOM | 78 | CD | ARG | 10 | 46.002 | 11.635 | 46.264 | 1.00 | 52.63 | AAAA | C |
| ATOM | 79 | HE | ARG | 10 | 45.082 | 12.226 | 45.284 | 1.00 | 59.27 | AAAA | H |
| ATOM | 81 | CE | ARG | 10 | 44.269 | 13.262 | 45.498 | 1.00 | 56.22 | AAAA | C |
| ATOM | 82 | NH1 | ARG | 10 | 44.153 | 13.891 | 46.666 | 1.00 | 55.14 | AAAA | H |
| ATOM | 95 | NH2 | ARG | 10 | 43.455 | 13.803 | 44.602 | 1.00 | 52.29 | AAAA | H |
| ATOM | 98 | C | ARG | 10 | 47.019 | 7.373 | 46.492 | 1.00 | 57.23 | AAAA | C |
| ATOM | 89 | O | ARG | 10 | 48.240 | 7.288 | 46.281 | 1.00 | 56.32 | AAAA | O |
| ATOM | 90 | H | ASN | 11 | 46.248 | 6.654 | 45.629 | 1.00 | 57.23 | AAAA | N |
| ATOM | 92 | CA | ASN | 11 | 46.800 | 5.917 | 44.494 | 1.00 | 50.73 | AAAA | C |
| ATOM | 93 | CB | ASN | 11 | 47.704 | 6.798 | 43.671 | 1.00 | 44.65 | AAAA | C |
| ATOM | 94 | CG | ASN | 11 | 46.878 | 7.732 | 42.829 | 1.00 | 50.72 | AAAA | C |
| ATOM | 95 | OD1 | ASN | 11 | 45.749 | 7.451 | 42.403 | 1.00 | 72.59 | AAAA | O |
| ATOM | 96 | ND2 | ASN | 11 | 47.499 | 8.869 | 42.587 | 1.00 | 54.38 | AAAA | H |
| ATOM | 99 | C | ASN | 11 | 47.635 | 4.736 | 44.915 | 1.00 | 53.07 | AAAA | C |
| ATOM | 100 | O | ASN | 11 | 47.303 | 3.701 | 44.347 | 1.00 | 51.95 | AAAA | O |
| ATOM | 101 | H | ASP | 12 | 48.566 | 4.822 | 45.878 | 1.00 | 50.96 | AAAA | H |
| ATOM | 103 | CA | ASP | 12 | 49.204 | 3.570 | 46.263 | 1.00 | 55.44 | AAAA | C |

| | | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 104 | CB | ASP | 12 | 50.568 | 3.568 | 45.758 | 1.00 | 66.47 | AAAA | C |
| ATOM | 105 | CG | ASP | 12 | 50.879 | 4.026 | 44.314 | 1.00 | 68.25 | AAAA | C |
| ATOM | 106 | OD1 | ASP | 12 | 50.441 | 3.185 | 43.457 | 1.00 | 58.31 | AAAA | O |
| ATOM | 107 | OD2 | ASP | 12 | 51.391 | 5.120 | 43.989 | 1.00 | 70.56 | AAAA | O |
| ATOM | 108 | C | ASP | 12 | 49.061 | 3.322 | 47.758 | 1.00 | 59.23 | AAAA | C |
| ATOM | 109 | O | ASP | 12 | 49.687 | 3.849 | 48.711 | 1.00 | 59.65 | AAAA | O |
| ATOM | 110 | H | TYR | 13 | 48.411 | 2.187 | 48.036 | 1.00 | 59.64 | AAAA | N |
| ATOM | 112 | CA | TYR | 13 | 48.328 | 1.672 | 49.397 | 1.00 | 64.06 | AAAA | C |
| ATOM | 113 | CB | TYR | 13 | 47.968 | 0.196 | 49.409 | 1.00 | 64.56 | AAAA | C |
| ATOM | 114 | CG | TYR | 13 | 47.467 | -0.357 | 50.721 | 1.00 | 69.18 | AAAA | C |
| ATOM | 115 | CD1 | TYR | 13 | 46.216 | -0.024 | 51.248 | 1.00 | 72.71 | AAAA | C |
| ATOM | 116 | CE1 | TYR | 13 | 45.746 | -0.541 | 52.450 | 1.00 | 71.51 | AAAA | C |
| ATOM | 117 | CD2 | TYR | 13 | 48.233 | -1.247 | 51.457 | 1.00 | 70.36 | AAAA | C |
| ATOM | 118 | CE2 | TYR | 13 | 47.788 | -1.778 | 52.661 | 1.00 | 71.64 | AAAA | C |
| ATOM | 119 | CC | TYR | 13 | 46.542 | -1.420 | 53.160 | 1.00 | 71.31 | AAAA | C |
| ATOM | 120 | OH | TYR | 13 | 46.144 | -1.977 | 54.358 | 1.00 | 63.25 | AAAA | O |
| ATOM | 122 | C | TYR | 13 | 49.622 | 1.839 | 50.198 | 1.00 | 65.99 | AAAA | C |
| ATOM | 123 | O | TYR | 13 | 49.621 | 2.321 | 51.354 | 1.00 | 65.01 | AAAA | O |
| ATOM | 124 | H | GLN | 14 | 50.786 | 1.541 | 49.594 | 1.00 | 63.51 | AAAA | N |
| ATOM | 126 | CA | GLN | 14 | 52.078 | 1.681 | 50.218 | 1.00 | 63.51 | AAAA | C |
| ATOM | 127 | CB | GLN | 14 | 53.174 | 1.318 | 49.219 | 1.00 | 68.37 | AAAA | C |
| ATOM | 128 | CG | GLN | 14 | 52.863 | -0.078 | 48.686 | 1.00 | 84.62 | AAAA | C |
| ATOM | 129 | CD | GLN | 14 | 53.990 | -0.515 | 47.754 | 1.00 | 92.28 | AAAA | C |
| ATOM | 130 | OE1 | GLN | 14 | 53.945 | -0.161 | 46.573 | 1.00 | 94.82 | AAAA | O |
| ATOM | 131 | NE2 | GLN | 14 | 54.920 | -1.254 | 48.361 | 1.00 | 98.03 | AAAA | N |
| ATOM | 134 | C | GLN | 14 | 52.434 | 3.058 | 50.753 | 1.00 | 61.62 | AAAA | C |
| ATOM | 135 | O | GLN | 14 | 53.266 | 3.292 | 51.644 | 1.00 | 62.09 | AAAA | O |
| ATOM | 136 | H | GLN | 15 | 51.628 | 4.038 | 50.349 | 1.00 | 57.02 | AAAA | H |
| ATOM | 138 | CA | GLN | 15 | 51.724 | 5.399 | 50.834 | 1.00 | 51.71 | AAAA | C |
| ATOM | 139 | CB | GLN | 15 | 50.861 | 6.220 | 49.911 | 1.00 | 43.75 | AAAA | C |
| ATOM | 140 | CG | GLN | 15 | 51.566 | 6.605 | 48.648 | 1.00 | 59.65 | AAAA | C |
| ATOM | 141 | CD | GLN | 15 | 51.554 | 8.105 | 48.428 | 1.00 | 72.96 | AAAA | C |
| ATOM | 142 | OE1 | GLN | 15 | 51.168 | 9.005 | 49.184 | 1.00 | 80.58 | AAAA | O |
| ATOM | 143 | NE2 | GLN | 15 | 52.016 | 8.378 | 47.211 | 1.00 | 74.17 | AAAA | H |
| ATOM | 146 | C | GLN | 15 | 51.219 | 5.530 | 52.259 | 1.00 | 50.15 | AAAA | C |
| ATOM | 147 | O | GLN | 15 | 51.576 | 6.500 | 52.940 | 1.00 | 49.04 | AAAA | O |
| ATOM | 148 | H | LEU | 16 | 50.440 | 4.535 | 52.688 | 1.00 | 46.22 | AAAA | H |
| ATOM | 150 | CA | LEU | 16 | 49.913 | 4.449 | 54.019 | 1.00 | 45.52 | AAAA | C |
| ATOM | 151 | CB | LEU | 16 | 48.950 | 3.295 | 54.159 | 1.00 | 37.73 | AAAA | C |
| ATOM | 152 | CG | LEU | 16 | 47.502 | 3.425 | 53.707 | 1.00 | 41.40 | AAAA | C |
| ATOM | 153 | CD1 | LEU | 16 | 46.837 | 2.063 | 53.790 | 1.00 | 42.43 | AAAA | C |
| ATOM | 154 | CD2 | LEU | 16 | 46.687 | 4.424 | 54.545 | 1.00 | 35.93 | AAAA | C |
| ATOM | 155 | O | LEU | 16 | 51.042 | 4.280 | 55.039 | 1.00 | 51.52 | AAAA | C |
| ATOM | 156 | C | LEU | 16 | 50.913 | 4.601 | 56.235 | 1.00 | 52.53 | AAAA | O |
| ATOM | 157 | H | LYS | 17 | 52.252 | 3.936 | 54.560 | 1.00 | 51.01 | AAAA | H |
| ATOM | 159 | CA | LYS | 17 | 53.422 | 3.914 | 55.404 | 1.00 | 50.73 | AAAA | C |
| ATOM | 160 | CB | LYS | 17 | 54.609 | 3.252 | 54.737 | 1.00 | 56.10 | AAAA | C |
| ATOM | 161 | CG | LYS | 17 | 54.539 | 1.733 | 54.831 | 1.00 | 62.40 | AAAA | C |
| ATOM | 162 | CD | LYS | 17 | 54.769 | 1.278 | 53.387 | 1.00 | 63.95 | AAAA | C |
| ATOM | 163 | CE | LYS | 17 | 55.316 | -0.141 | 53.426 | 1.00 | 68.40 | AAAA | C |
| ATOM | 164 | NE | LYS | 17 | 56.537 | -0.225 | 52.554 | 1.00 | 73.93 | AAAA | H |
| ATOM | 169 | C | LYS | 17 | 53.944 | 5.270 | 55.852 | 1.00 | 44.75 | AAAA | C |
| ATOM | 169 | O | LYS | 17 | 54.492 | 5.262 | 56.933 | 1.00 | 39.39 | AAAA | O |
| ATOM | 170 | H | ARG | 18 | 53.524 | 6.344 | 55.201 | 1.00 | 41.15 | AAAA | H |
| ATOM | 172 | CA | ARG | 18 | 53.827 | 7.673 | 55.676 | 1.00 | 43.01 | AAAA | C |
| ATOM | 173 | CB | ARG | 18 | 53.250 | 8.702 | 54.704 | 1.00 | 43.97 | AAAA | C |
| ATOM | 174 | CG | ARG | 18 | 53.888 | 8.764 | 53.333 | 1.00 | 53.60 | AAAA | C |
| ATOM | 175 | CD | ARG | 18 | 52.964 | 9.362 | 52.269 | 1.00 | 60.34 | AAAA | C |
| ATOM | 176 | NE | ARG | 18 | 52.528 | 10.703 | 52.650 | 1.00 | 50.00 | AAAA | H |
| ATOM | 178 | CC | ARG | 18 | 51.628 | 11.444 | 52.021 | 1.00 | 48.86 | AAAA | C |
| ATOM | 179 | NH1 | ARG | 18 | 51.068 | 10.941 | 50.943 | 1.00 | 47.96 | AAAA | H |
| ATOM | 182 | NH2 | ARG | 18 | 51.377 | 12.656 | 52.555 | 1.00 | 43.72 | AAAA | H |
| ATOM | 185 | C | ARG | 18 | 53.268 | 7.924 | 57.077 | 1.00 | 44.03 | AAAA | C |
| ATOM | 186 | O | ARG | 18 | 53.402 | 9.010 | 57.644 | 1.00 | 45.53 | AAAA | O |
| ATOM | 187 | H | LEU | 19 | 52.445 | 7.069 | 57.632 | 1.00 | 46.36 | AAAA | H |
| ATOM | 189 | CA | LEU | 19 | 51.653 | 7.282 | 58.794 | 1.00 | 50.25 | AAAA | C |
| ATOM | 190 | CB | LEU | 19 | 50.186 | 6.924 | 58.674 | 1.00 | 50.83 | AAAA | C |
| ATOM | 191 | CG | LEU | 19 | 49.202 | 7.371 | 57.608 | 1.00 | 46.43 | AAAA | C |
| ATOM | 192 | CD1 | LEU | 19 | 47.846 | 6.743 | 57.852 | 1.00 | 22.57 | AAAA | C |
| ATOM | 193 | CD2 | LEU | 19 | 49.018 | 8.966 | 57.495 | 1.00 | 45.88 | AAAA | C |
| ATOM | 194 | C | LEU | 19 | 52.210 | 6.428 | 59.912 | 1.00 | 49.87 | AAAA | C |
| ATOM | 195 | O | LEU | 19 | 51.870 | 6.810 | 61.030 | 1.00 | 51.54 | AAAA | O |
| ATOM | 196 | H | GLU | 20 | 53.270 | 5.708 | 59.652 | 1.00 | 49.35 | AAAA | H |
| ATOM | 198 | CA | GLU | 20 | 53.819 | 4.933 | 60.679 | 1.00 | 49.60 | AAAA | C |
| ATOM | 199 | CB | GLU | 20 | 54.876 | 3.960 | 59.982 | 1.00 | 57.91 | AAAA | C |
| ATOM | 200 | CG | GLU | 20 | 55.893 | 4.940 | 59.272 | 1.00 | 70.16 | AAAA | C |
| ATOM | 201 | CD | GLU | 20 | 57.095 | 4.077 | 58.757 | 1.00 | 69.35 | AAAA | C |
| ATOM | 202 | OE1 | GLU | 20 | 58.123 | 4.795 | 58.722 | 1.00 | 71.39 | AAAA | O |
| ATOM | 203 | OE2 | GLU | 20 | 56.993 | 2.885 | 58.420 | 1.00 | 72.94 | AAAA | O |
| ATOM | 204 | C | GLU | 20 | 54.310 | 5.417 | 61.989 | 1.00 | 43.55 | AAAA | C |
| ATOM | 205 | O | GLU | 20 | 54.301 | 4.652 | 62.937 | 1.00 | 40.01 | AAAA | O |
| ATOM | 206 | H | ASN | 21 | 54.633 | 6.659 | 62.207 | 1.00 | 41.06 | AAAA | H |
| ATOM | 208 | CA | ASN | 21 | 55.054 | 7.204 | 63.454 | 1.00 | 47.17 | AAAA | C |
| ATOM | 209 | C | ASN | 21 | 54.066 | 8.141 | 64.108 | 1.00 | 49.76 | AAAA | C |
| ATOM | 210 | O | ASN | 21 | 54.228 | 9.456 | 65.303 | 1.00 | 48.10 | AAAA | O |

| | | | | | | | | | | | |
|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 211 | CP | ASN | 21 | 56.379 | 8.003 | 63.290 | 1.00 | 59.11 | AAAA | C |
| ATOM | 212 | CG | ASN | 21 | 57.413 | 7.051 | 62.796 | 1.00 | 68.38 | AAAA | C |
| ATOM | 213 | OD1 | ASN | 21 | 57.499 | 5.955 | 63.122 | 1.00 | 58.51 | AAAA | O |
| ATOM | 214 | ND2 | ASN | 21 | 58.348 | 7.469 | 61.890 | 1.00 | 77.90 | AAAA | N |
| ATOM | 216 | H | CYS | 22 | 53.129 | 8.711 | 63.351 | 1.00 | 47.44 | AAAA | H |
| ATOM | 218 | CA | CYS | 22 | 52.107 | 9.614 | 63.879 | 1.00 | 42.99 | AAAA | C |
| ATOM | 219 | C | CYS | 22 | 51.215 | 9.089 | 65.021 | 1.00 | 40.43 | AAAA | C |
| ATOM | 220 | O | CYS | 22 | 50.750 | 7.923 | 65.069 | 1.00 | 36.07 | AAAA | O |
| ATOM | 221 | CB | CYS | 22 | 51.182 | 9.921 | 62.690 | 1.00 | 44.82 | AAAA | C |
| ATOM | 222 | SG | CYS | 22 | 52.076 | 10.328 | 61.148 | 1.00 | 39.51 | AAAA | S |
| ATOM | 223 | H | THR | 23 | 51.287 | 9.801 | 66.137 | 1.00 | 36.24 | AAAA | H |
| ATOM | 225 | CA | THR | 23 | 50.339 | 9.482 | 67.204 | 1.00 | 43.51 | AAAA | C |
| ATOM | 226 | CB | THR | 23 | 50.944 | 9.481 | 68.593 | 1.00 | 41.38 | AAAA | C |
| ATOM | 227 | OG1 | THR | 23 | 51.410 | 10.843 | 68.822 | 1.00 | 51.21 | AAAA | O |
| ATOM | 229 | CG2 | THR | 23 | 52.110 | 8.571 | 68.838 | 1.00 | 33.83 | AAAA | C |
| ATOM | 230 | C | THR | 23 | 49.250 | 10.599 | 67.116 | 1.00 | 44.55 | AAAA | C |
| ATOM | 231 | O | THR | 23 | 48.085 | 10.414 | 67.481 | 1.00 | 45.95 | AAAA | O |
| ATOM | 232 | H | VAL | 24 | 49.646 | 11.797 | 66.689 | 1.00 | 33.03 | AAAA | H |
| ATOM | 234 | CA | VAL | 24 | 48.732 | 12.855 | 66.442 | 1.00 | 35.29 | AAAA | C |
| ATOM | 235 | CB | VAL | 24 | 48.925 | 13.979 | 67.456 | 1.00 | 30.60 | AAAA | C |
| ATOM | 236 | CG1 | VAL | 24 | 48.056 | 15.157 | 67.082 | 1.00 | 27.21 | AAAA | C |
| ATOM | 237 | CG2 | VAL | 24 | 48.656 | 13.566 | 68.886 | 1.00 | 25.37 | AAAA | C |
| ATOM | 238 | C | VAL | 24 | 48.895 | 13.447 | 65.043 | 1.00 | 41.52 | AAAA | C |
| ATOM | 239 | O | VAL | 24 | 49.987 | 13.963 | 64.791 | 1.00 | 44.40 | AAAA | O |
| ATOM | 240 | H | ILE | 25 | 47.855 | 13.450 | 64.203 | 1.00 | 40.13 | AAAA | N |
| ATOM | 242 | CA | ILE | 25 | 47.908 | 14.094 | 62.882 | 1.00 | 32.05 | AAAA | C |
| ATOM | 243 | CB | ILE | 25 | 47.113 | 13.299 | 61.853 | 1.00 | 25.85 | AAAA | C |
| ATOM | 244 | CG2 | ILE | 25 | 47.027 | 14.039 | 60.542 | 1.00 | 18.73 | AAAA | C |
| ATOM | 245 | CG1 | ILE | 25 | 47.677 | 11.896 | 61.705 | 1.00 | 29.80 | AAAA | C |
| ATOM | 246 | CD1 | ILE | 25 | 47.169 | 11.155 | 60.471 | 1.00 | 27.41 | AAAA | C |
| ATOM | 247 | C | ILE | 25 | 47.397 | 15.490 | 62.941 | 1.00 | 32.92 | AAAA | C |
| ATOM | 248 | O | ILE | 25 | 46.223 | 15.776 | 63.213 | 1.00 | 40.91 | AAAA | O |
| ATOM | 249 | H | GLU | 26 | 48.264 | 16.472 | 63.042 | 1.00 | 36.60 | AAAA | H |
| ATOM | 251 | CA | GLU | 26 | 47.832 | 17.847 | 63.226 | 1.00 | 29.24 | AAAA | C |
| ATOM | 252 | CB | GLU | 26 | 48.875 | 18.703 | 63.856 | 1.00 | 29.92 | AAAA | C |
| ATOM | 253 | CG | GLU | 26 | 49.490 | 20.144 | 64.116 | 1.00 | 38.06 | AAAA | C |
| ATOM | 254 | CD | GLU | 26 | 49.561 | 20.762 | 65.013 | 1.00 | 37.39 | AAAA | C |
| ATOM | 255 | OE1 | GLU | 26 | 50.654 | 20.937 | 64.489 | 1.00 | 41.56 | AAAA | O |
| ATOM | 256 | OE2 | GLU | 26 | 49.571 | 21.175 | 65.182 | 1.00 | 49.16 | AAAA | O |
| ATOM | 257 | C | GLU | 26 | 47.413 | 18.376 | 61.969 | 1.00 | 37.79 | AAAA | C |
| ATOM | 258 | O | GLU | 26 | 48.161 | 19.069 | 61.181 | 1.00 | 39.69 | AAAA | O |
| ATOM | 259 | H | GLY | 27 | 46.117 | 19.104 | 61.582 | 1.00 | 37.28 | AAAA | H |
| ATOM | 261 | CA | GLY | 27 | 45.498 | 18.503 | 60.320 | 1.00 | 31.17 | AAAA | C |
| ATOM | 262 | C | GLY | 27 | 44.531 | 17.400 | 59.893 | 1.00 | 33.72 | AAAA | C |
| ATOM | 263 | O | GLY | 27 | 43.988 | 16.715 | 59.775 | 1.00 | 33.29 | AAAA | O |
| ATOM | 264 | H | TYR | 28 | 44.304 | 17.209 | 59.604 | 1.00 | 29.24 | AAAA | H |
| ATOM | 266 | CA | TYR | 28 | 43.318 | 16.189 | 59.253 | 1.00 | 28.93 | AAAA | C |
| ATOM | 267 | CB | TYR | 28 | 42.403 | 16.794 | 57.217 | 1.00 | 31.53 | AAAA | C |
| ATOM | 268 | CG | TYR | 28 | 43.058 | 17.256 | 55.962 | 1.00 | 31.78 | AAAA | C |
| ATOM | 269 | CD1 | TYR | 28 | 43.704 | 16.355 | 55.116 | 1.00 | 36.07 | AAAA | C |
| ATOM | 270 | OE1 | TYR | 28 | 44.361 | 16.706 | 53.967 | 1.00 | 29.91 | AAAA | C |
| ATOM | 271 | OE2 | TYR | 28 | 43.130 | 19.572 | 55.606 | 1.00 | 30.99 | AAAA | C |
| ATOM | 272 | CE2 | TYR | 28 | 43.769 | 18.972 | 54.428 | 1.00 | 28.77 | AAAA | C |
| ATOM | 273 | CS | TYR | 28 | 44.367 | 18.021 | 53.652 | 1.00 | 31.53 | AAAA | C |
| ATOM | 274 | OH | TYR | 28 | 44.971 | 18.425 | 52.464 | 1.00 | 44.74 | AAAA | O |
| ATOM | 276 | C | TYR | 28 | 43.953 | 14.946 | 57.697 | 1.00 | 29.23 | AAAA | C |
| ATOM | 277 | O | TYR | 28 | 45.119 | 15.147 | 57.383 | 1.00 | 35.58 | AAAA | O |
| ATOM | 278 | H | LEU | 29 | 43.250 | 13.900 | 57.445 | 1.00 | 26.63 | AAAA | N |
| ATOM | 280 | CA | LEU | 29 | 43.764 | 12.730 | 56.803 | 1.00 | 29.83 | AAAA | C |
| ATOM | 281 | CB | LEU | 29 | 43.830 | 11.611 | 57.856 | 1.00 | 27.09 | AAAA | C |
| ATOM | 282 | CG | LEU | 29 | 44.212 | 10.258 | 57.242 | 1.00 | 31.90 | AAAA | C |
| ATOM | 283 | CD1 | LEU | 29 | 45.538 | 10.396 | 56.469 | 1.00 | 35.03 | AAAA | C |
| ATOM | 284 | CD2 | LEU | 29 | 44.551 | 9.203 | 58.290 | 1.00 | 25.05 | AAAA | C |
| ATOM | 285 | C | LEU | 29 | 42.897 | 12.342 | 55.616 | 1.00 | 33.84 | AAAA | C |
| ATOM | 286 | O | LEU | 29 | 41.689 | 12.165 | 55.806 | 1.00 | 43.29 | AAAA | O |
| ATOM | 287 | H | HIS | 30 | 43.389 | 12.285 | 54.395 | 1.00 | 35.95 | AAAA | H |
| ATOM | 289 | CA | HIS | 30 | 42.681 | 11.891 | 53.197 | 1.00 | 34.92 | AAAA | C |
| ATOM | 290 | CB | HIS | 30 | 42.893 | 12.801 | 52.027 | 1.00 | 32.85 | AAAA | C |
| ATOM | 291 | CG | HIS | 30 | 42.372 | 14.155 | 52.046 | 1.00 | 25.09 | AAAA | C |
| ATOM | 292 | CD2 | HIS | 30 | 41.519 | 14.753 | 52.907 | 1.00 | 40.88 | AAAA | C |
| ATOM | 293 | ND1 | HIS | 30 | 42.717 | 15.120 | 51.128 | 1.00 | 33.66 | AAAA | H |
| ATOM | 295 | CE1 | HIS | 30 | 42.080 | 16.281 | 51.444 | 1.00 | 31.33 | AAAA | C |
| ATOM | 296 | HE2 | HIS | 30 | 41.329 | 16.093 | 52.539 | 1.00 | 37.27 | AAAA | H |
| ATOM | 298 | C | HIS | 30 | 43.173 | 10.538 | 52.714 | 1.00 | 37.68 | AAAA | C |
| ATOM | 299 | O | HIS | 30 | 44.357 | 10.388 | 52.541 | 1.00 | 38.70 | AAAA | O |
| ATOM | 300 | H | ILE | 31 | 42.308 | 9.542 | 52.584 | 1.00 | 40.02 | AAAA | H |
| ATOM | 302 | CA | ILE | 31 | 42.750 | 8.271 | 51.992 | 1.00 | 39.47 | AAAA | C |
| ATOM | 303 | CB | ILE | 31 | 42.668 | 7.204 | 53.063 | 1.00 | 37.95 | AAAA | C |
| ATOM | 304 | CG2 | ILE | 31 | 43.161 | 5.830 | 52.651 | 1.00 | 23.86 | AAAA | C |
| ATOM | 305 | CG1 | ILE | 31 | 43.481 | 7.555 | 54.335 | 1.00 | 41.66 | AAAA | C |
| ATOM | 306 | CD1 | ILE | 31 | 43.170 | 6.575 | 55.473 | 1.00 | 28.22 | AAAA | C |
| ATOM | 307 | C | ILE | 31 | 41.884 | 8.044 | 50.755 | 1.00 | 46.52 | AAAA | C |
| ATOM | 308 | O | ILE | 31 | 40.753 | 7.589 | 50.827 | 1.00 | 43.56 | AAAA | O |
| ATOM | 309 | H | LEU | 32 | 42.314 | 8.489 | 49.556 | 1.00 | 49.89 | AAAA | H |
| ATOM | 311 | CA | LEU | 32 | 41.484 | 8.235 | 48.380 | 1.00 | 49.77 | AAAA | C |

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|------|-----|-----|-----|----|--------|---------|--------|------|--------|------|---|
| ATOH | 312 | CB | LEU | 32 | 41.127 | 9.515 | 47.603 | 1.00 | 47.48 | AAAA | C |
| ATOH | 313 | CG | LEU | 32 | 42.091 | 10.688 | 47.562 | 1.00 | 45.33 | AAAA | C |
| ATOH | 314 | CD1 | LEU | 32 | 41.517 | 11.812 | 46.673 | 1.00 | 35.77 | AAAA | C |
| ATOH | 315 | CD2 | LEU | 32 | 42.371 | 11.229 | 48.960 | 1.00 | 49.18 | AAAA | C |
| ATOH | 316 | C | LEU | 32 | 42.136 | 7.296 | 47.353 | 1.00 | 51.00 | AAAA | C |
| ATOH | 317 | O | LEU | 32 | 43.338 | 7.370 | 47.186 | 1.00 | 41.36 | AAAA | O |
| ATOH | 318 | H | LEU | 33 | 41.270 | 6.722 | 46.497 | 1.00 | 50.74 | AAAA | H |
| ATOH | 320 | CA | LEU | 33 | 41.602 | 6.175 | 45.197 | 1.00 | 49.92 | AAAA | C |
| ATOH | 321 | CB | LEU | 33 | 42.091 | 7.262 | 44.182 | 1.00 | 34.83 | AAAA | C |
| ATOH | 322 | CG | LEU | 33 | 41.233 | 8.537 | 44.164 | 1.00 | 33.92 | AAAA | C |
| ATOH | 323 | CD1 | LEU | 33 | 41.892 | 9.587 | 43.298 | 1.00 | 37.49 | AAAA | C |
| ATOH | 324 | CD2 | LEU | 33 | 39.823 | 8.313 | 43.644 | 1.00 | 33.01 | AAAA | C |
| ATOH | 325 | C | LEU | 33 | 42.618 | 5.073 | 45.287 | 1.00 | 48.35 | AAAA | C |
| ATOH | 326 | O | LEU | 33 | 43.580 | 5.077 | 44.538 | 1.00 | 54.14 | AAAA | O |
| ATOH | 327 | H | ILE | 34 | 42.543 | 4.212 | 46.254 | 1.00 | 47.61 | AAAA | H |
| ATOH | 329 | CA | ILE | 34 | 43.523 | 3.184 | 46.540 | 1.00 | 51.70 | AAAA | C |
| ATOH | 330 | CB | ILE | 34 | 44.101 | 3.346 | 47.963 | 1.00 | 57.98 | AAAA | C |
| ATOH | 331 | CG2 | ILE | 34 | 44.538 | 2.043 | 48.600 | 1.00 | 48.98 | AAAA | C |
| ATOH | 332 | CG1 | ILE | 34 | 45.267 | 4.371 | 47.967 | 1.00 | 46.70 | AAAA | C |
| ATOH | 333 | CD1 | ILE | 34 | 45.561 | 4.704 | 49.439 | 1.00 | 66.47 | AAAA | C |
| ATOH | 334 | C | ILE | 34 | 42.829 | 1.844 | 46.408 | 1.00 | 59.85 | AAAA | C |
| ATOH | 335 | O | ILE | 34 | 41.726 | 1.531 | 46.856 | 1.00 | 60.11 | AAAA | O |
| ATOH | 336 | H | SER | 35 | 43.622 | 0.833 | 46.013 | 1.00 | 67.79 | AAAA | H |
| ATOH | 338 | CA | SER | 35 | 43.048 | -0.511 | 45.922 | 1.00 | 68.80 | AAAA | C |
| ATOH | 339 | CB | SER | 35 | 42.767 | -0.882 | 44.469 | 1.00 | 64.16 | AAAA | C |
| ATOH | 340 | OG | SER | 35 | 41.731 | -1.846 | 44.498 | 1.00 | 75.76 | AAAA | O |
| ATOH | 342 | C | SER | 35 | 43.928 | -1.564 | 46.537 | 1.00 | 70.73 | AAAA | C |
| ATOH | 343 | O | SER | 35 | 44.885 | -1.954 | 45.909 | 1.00 | 73.65 | AAAA | O |
| ATOH | 344 | N | LYS | 36 | 43.687 | -2.017 | 47.740 | 1.00 | 74.75 | AAAA | N |
| ATOH | 346 | CA | LYS | 36 | 44.465 | -3.014 | 48.421 | 1.00 | 76.09 | AAAA | C |
| ATOH | 347 | CB | LYS | 36 | 44.046 | -3.131 | 49.885 | 1.00 | 81.22 | AAAA | C |
| ATOH | 348 | CG | LYS | 36 | 45.147 | -3.654 | 50.775 | 1.00 | 78.87 | AAAA | C |
| ATOH | 349 | CD | LYS | 36 | 44.693 | -4.575 | 51.887 | 1.00 | 81.39 | AAAA | C |
| ATOH | 350 | CE | LYS | 36 | 44.890 | -6.025 | 51.492 | 1.00 | 89.39 | AAAA | C |
| ATOH | 351 | HC | LYS | 36 | 44.371 | -6.939 | 52.506 | 1.00 | 91.63 | AAAA | H |
| ATOH | 355 | C | LYS | 36 | 44.252 | -4.362 | 47.753 | 1.00 | 81.41 | AAAA | C |
| ATOH | 356 | O | LYS | 36 | 43.145 | -4.772 | 47.451 | 1.00 | 78.20 | AAAA | O |
| ATOH | 357 | H | ALA | 37 | 45.371 | -5.080 | 47.615 | 1.00 | 88.27 | AAAA | H |
| ATOH | 359 | CA | ALA | 37 | 45.361 | -6.336 | 46.986 | 1.00 | 90.10 | AAAA | C |
| ATOH | 360 | CB | ALA | 37 | 46.700 | -6.655 | 46.327 | 1.00 | 95.49 | AAAA | C |
| ATOH | 361 | C | ALA | 37 | 45.111 | -7.473 | 47.995 | 1.00 | 92.36 | AAAA | C |
| ATOH | 362 | O | ALA | 37 | 45.668 | -7.627 | 49.012 | 1.00 | 92.35 | AAAA | O |
| ATOH | 363 | H | SER | 38 | 44.031 | -9.301 | 47.622 | 1.00 | 94.31 | AAAA | H |
| ATOH | 365 | CA | SER | 38 | 43.528 | -9.352 | 49.484 | 1.00 | 95.70 | AAAA | C |
| ATOH | 366 | CB | SER | 38 | 42.405 | -10.164 | 47.858 | 1.00 | 97.44 | AAAA | C |
| ATOH | 367 | OG | SER | 38 | 42.361 | -11.176 | 49.814 | 1.00 | 103.49 | AAAA | O |
| ATOH | 369 | C | SER | 38 | 44.702 | -10.263 | 48.821 | 1.00 | 96.87 | AAAA | C |
| ATOH | 370 | O | SER | 38 | 44.761 | -10.778 | 49.924 | 1.00 | 98.06 | AAAA | O |
| ATOH | 371 | H | ASP | 39 | 45.884 | -10.415 | 47.952 | 1.00 | 97.99 | AAAA | H |
| ATOH | 373 | CA | ASP | 39 | 46.821 | -11.148 | 47.990 | 1.00 | 99.19 | AAAA | C |
| ATOH | 374 | CB | ASP | 39 | 47.579 | -11.050 | 46.652 | 1.00 | 102.13 | AAAA | C |
| ATOH | 375 | CG | ASP | 39 | 47.496 | -12.397 | 45.948 | 0.01 | 101.22 | AAAA | C |
| ATOH | 376 | CD1 | ASP | 39 | 46.644 | -12.978 | 45.623 | 0.01 | 101.42 | AAAA | O |
| ATOH | 377 | CD2 | ASP | 39 | 48.933 | -12.848 | 45.718 | 0.01 | 101.41 | AAAA | O |
| ATOH | 378 | C | ASP | 39 | 47.660 | -10.564 | 49.105 | 1.00 | 99.40 | AAAA | C |
| ATOH | 379 | O | ASP | 39 | 47.692 | -11.056 | 50.224 | 1.00 | 99.15 | AAAA | O |
| ATOH | 380 | H | TYR | 40 | 48.354 | -9.479 | 48.818 | 1.00 | 100.96 | AAAA | H |
| ATOH | 382 | CA | TYR | 40 | 49.120 | -9.706 | 49.802 | 1.00 | 101.16 | AAAA | C |
| ATOH | 383 | CB | TYR | 40 | 49.511 | -7.393 | 49.130 | 1.00 | 103.67 | AAAA | C |
| ATOH | 384 | CG | TYR | 40 | 50.159 | -6.281 | 49.887 | 1.00 | 107.81 | AAAA | C |
| ATOH | 385 | CD1 | TYR | 40 | 50.931 | -5.325 | 49.228 | 1.00 | 109.56 | AAAA | C |
| ATOH | 386 | CE1 | TYR | 40 | 51.540 | -4.280 | 49.910 | 1.00 | 109.67 | AAAA | C |
| ATOH | 387 | CD2 | TYR | 40 | 50.044 | -6.115 | 51.254 | 1.00 | 109.28 | AAAA | C |
| ATOH | 388 | CE2 | TYR | 40 | 50.618 | -5.102 | 51.976 | 1.00 | 109.83 | AAAA | C |
| ATOH | 389 | CG | TYR | 40 | 51.372 | -4.181 | 51.276 | 1.00 | 110.16 | AAAA | C |
| ATOH | 390 | OH | TYR | 40 | 51.999 | -3.127 | 51.893 | 1.00 | 109.84 | AAAA | O |
| ATOH | 392 | C | TYR | 40 | 48.343 | -8.529 | 51.100 | 1.00 | 99.10 | AAAA | C |
| ATOH | 393 | O | TYR | 40 | 47.168 | -8.182 | 51.183 | 1.00 | 99.05 | AAAA | O |
| ATOH | 394 | H | LYS | 41 | 49.041 | -8.653 | 52.218 | 1.00 | 98.62 | AAAA | H |
| ATOH | 396 | CA | LYS | 41 | 48.443 | -8.549 | 53.546 | 1.00 | 100.30 | AAAA | C |
| ATOH | 397 | CB | LYS | 41 | 49.385 | -9.160 | 54.599 | 1.00 | 104.42 | AAAA | C |
| ATOH | 398 | CG | LYS | 41 | 49.218 | -10.649 | 54.814 | 0.01 | 101.06 | AAAA | C |
| ATOH | 399 | CD | LYS | 41 | 47.776 | -11.107 | 54.919 | 0.01 | 100.66 | AAAA | C |
| ATOH | 400 | CE | LYS | 41 | 47.205 | -10.880 | 56.308 | 0.01 | 99.86 | AAAA | C |
| ATOH | 401 | HC | LYS | 41 | 47.982 | -11.728 | 57.328 | 0.01 | 99.62 | AAAA | H |
| ATOH | 405 | C | LYS | 41 | 48.035 | -7.136 | 53.947 | 1.00 | 98.99 | AAAA | C |
| ATOH | 406 | O | LYS | 41 | 47.615 | -6.371 | 53.057 | 1.00 | 103.33 | AAAA | O |
| ATOH | 407 | H | SER | 42 | 48.198 | -6.754 | 55.221 | 1.00 | 91.75 | AAAA | H |
| ATOH | 409 | CA | SER | 42 | 47.825 | -5.412 | 55.604 | 1.00 | 85.06 | AAAA | C |
| ATOH | 410 | CB | SER | 42 | 46.385 | -5.520 | 56.147 | 1.00 | 95.33 | AAAA | C |
| ATOH | 411 | OG | SER | 42 | 46.547 | -6.140 | 57.426 | 1.00 | 104.63 | AAAA | O |
| ATOH | 413 | C | SER | 42 | 48.628 | -4.715 | 56.687 | 1.00 | 80.78 | AAAA | C |
| ATOH | 414 | O | SER | 42 | 49.326 | -5.259 | 57.538 | 1.00 | 81.03 | AAAA | O |
| ATOH | 415 | H | TYR | 43 | 48.495 | -3.395 | 56.676 | 1.00 | 73.03 | AAAA | H |
| ATOH | 417 | CA | TYR | 43 | 49.069 | -2.498 | 57.635 | 1.00 | 67.25 | AAAA | C |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATON | 419 | CB | TYR | 43 | 49.086 | -1.119 | 56.965 | 1.00 | 65.37 | AAAA | C |
| ATON | 419 | CG | TYR | 43 | 49.953 | -1.021 | 55.727 | 1.00 | 63.92 | AAAA | C |
| ATON | 420 | CD1 | TYR | 43 | 50.931 | -1.935 | 55.406 | 1.00 | 63.87 | AAAA | C |
| ATON | 421 | CE1 | TYR | 43 | 51.698 | -1.781 | 54.274 | 1.00 | 66.09 | AAAA | C |
| ATON | 422 | CD2 | TYR | 43 | 49.770 | 0.050 | 54.870 | 1.00 | 63.30 | AAAA | C |
| ATON | 423 | CE2 | TYR | 43 | 50.536 | 0.214 | 53.728 | 1.00 | 67.62 | AAAA | C |
| ATON | 424 | CS | TYR | 43 | 51.508 | -0.712 | 53.432 | 1.00 | 66.94 | AAAA | C |
| ATON | 425 | OH | TYR | 43 | 52.262 | -0.563 | 52.305 | 1.00 | 65.23 | AAAA | O |
| ATON | 427 | C | TYR | 43 | 48.248 | -2.381 | 58.925 | 1.00 | 64.88 | AAAA | C |
| ATON | 428 | O | TYR | 43 | 47.088 | -2.851 | 59.030 | 1.00 | 62.90 | AAAA | O |
| ATON | 429 | H | ARG | 44 | 48.782 | -1.567 | 59.825 | 1.00 | 57.88 | AAAA | N |
| ATON | 431 | CA | ARG | 44 | 48.019 | -1.285 | 61.039 | 1.00 | 56.45 | AAAA | C |
| ATON | 432 | CB | ARG | 44 | 47.842 | -2.611 | 61.760 | 1.00 | 46.51 | AAAA | C |
| ATON | 433 | CS | ARG | 44 | 47.815 | -2.375 | 63.244 | 1.00 | 54.66 | AAAA | C |
| ATON | 434 | CD | ARG | 44 | 46.985 | -3.327 | 63.986 | 1.00 | 58.54 | AAAA | C |
| ATON | 435 | HE | ARG | 44 | 47.090 | -2.927 | 65.403 | 1.00 | 69.56 | AAAA | N |
| ATON | 437 | CE | ARG | 44 | 46.464 | -3.536 | 66.395 | 1.00 | 64.82 | AAAA | C |
| ATON | 438 | HH1 | ARG | 44 | 45.644 | -4.529 | 66.132 | 1.00 | 61.63 | AAAA | N |
| ATON | 441 | HH2 | ARG | 44 | 46.674 | -3.139 | 67.628 | 1.00 | 66.03 | AAAA | N |
| ATON | 444 | C | ARG | 44 | 48.811 | -0.285 | 61.845 | 1.00 | 55.59 | AAAA | C |
| ATON | 445 | O | ARG | 44 | 49.916 | -0.552 | 62.320 | 1.00 | 58.43 | AAAA | O |
| ATON | 446 | H | PHE | 45 | 48.276 | 0.866 | 62.139 | 1.00 | 51.13 | AAAA | N |
| ATON | 448 | CA | PHE | 45 | 48.865 | 1.944 | 62.863 | 1.00 | 45.94 | AAAA | C |
| ATON | 449 | CB | PHE | 45 | 48.774 | 3.249 | 61.978 | 1.00 | 35.89 | AAAA | C |
| ATON | 450 | CG | PHE | 45 | 49.106 | 2.937 | 60.554 | 1.00 | 30.29 | AAAA | C |
| ATON | 451 | CD1 | PHE | 45 | 50.373 | 3.051 | 59.998 | 1.00 | 45.72 | AAAA | C |
| ATON | 452 | CD2 | PHE | 45 | 48.127 | 2.428 | 59.728 | 1.00 | 35.95 | AAAA | C |
| ATON | 453 | CE1 | PHE | 45 | 50.653 | 2.715 | 58.672 | 1.00 | 47.76 | AAAA | C |
| ATON | 454 | CE2 | PHE | 45 | 48.358 | 2.096 | 58.406 | 1.00 | 39.92 | AAAA | C |
| ATON | 455 | CS | PHE | 45 | 49.612 | 2.244 | 57.867 | 1.00 | 46.44 | AAAA | C |
| ATON | 456 | C | PHE | 45 | 48.181 | 2.123 | 64.203 | 1.00 | 41.65 | AAAA | C |
| ATON | 457 | O | PHE | 45 | 47.708 | 3.223 | 64.475 | 1.00 | 40.99 | AAAA | O |
| ATON | 459 | H | PRO | 46 | 48.494 | 1.338 | 65.212 | 1.00 | 43.20 | AAAA | N |
| ATON | 459 | CD | PRO | 46 | 49.300 | 0.097 | 65.132 | 1.00 | 47.74 | AAAA | C |
| ATON | 460 | CA | PRO | 46 | 49.032 | 1.530 | 66.560 | 1.00 | 43.34 | AAAA | C |
| ATON | 461 | CB | PRO | 46 | 48.514 | 0.319 | 67.380 | 1.00 | 44.92 | AAAA | C |
| ATON | 462 | CG | PRO | 46 | 49.404 | -0.464 | 66.514 | 1.00 | 45.48 | AAAA | C |
| ATON | 463 | C | PRO | 46 | 49.558 | 2.768 | 67.233 | 1.00 | 41.30 | AAAA | C |
| ATON | 464 | O | PRO | 46 | 49.329 | 2.930 | 68.443 | 1.00 | 44.57 | AAAA | O |
| ATON | 466 | H | LYS | 47 | 49.450 | 3.533 | 66.676 | 1.00 | 39.33 | AAAA | N |
| ATON | 467 | CA | LYS | 47 | 49.991 | 4.679 | 67.362 | 1.00 | 38.10 | AAAA | C |
| ATON | 468 | CB | LYS | 47 | 51.379 | 4.981 | 66.852 | 1.00 | 48.07 | AAAA | C |
| ATON | 469 | CG | LYS | 47 | 52.032 | 3.995 | 65.902 | 1.00 | 67.95 | AAAA | C |
| ATON | 470 | CD | LYS | 47 | 53.563 | 3.976 | 65.891 | 1.00 | 61.33 | AAAA | C |
| ATON | 471 | CE | LYS | 47 | 54.115 | 4.649 | 67.147 | 1.00 | 72.19 | AAAA | C |
| ATON | 472 | HC | LYS | 47 | 54.024 | 6.132 | 66.874 | 1.00 | 79.29 | AAAA | N |
| ATON | 476 | C | LYS | 47 | 49.014 | 5.849 | 67.195 | 1.00 | 39.76 | AAAA | C |
| ATON | 477 | O | LYS | 47 | 49.189 | 6.827 | 67.952 | 1.00 | 35.45 | AAAA | O |
| ATON | 478 | H | LEU | 48 | 49.300 | 5.986 | 66.053 | 1.00 | 36.45 | AAAA | N |
| ATON | 480 | CA | LEU | 49 | 47.370 | 7.004 | 65.800 | 1.00 | 40.40 | AAAA | C |
| ATON | 481 | CB | LEU | 49 | 46.823 | 6.919 | 64.389 | 1.00 | 28.59 | AAAA | C |
| ATON | 482 | CG | LEU | 49 | 45.947 | 7.967 | 63.787 | 1.00 | 31.04 | AAAA | C |
| ATON | 483 | CD1 | LEU | 48 | 46.637 | 9.310 | 63.878 | 1.00 | 36.96 | AAAA | C |
| ATON | 484 | CD2 | LEU | 48 | 45.591 | 7.738 | 62.294 | 1.00 | 34.49 | AAAA | C |
| ATON | 485 | C | LEU | 48 | 46.186 | 7.022 | 66.807 | 1.00 | 42.21 | AAAA | C |
| ATON | 486 | O | LEU | 48 | 45.271 | 6.187 | 66.863 | 1.00 | 36.48 | AAAA | O |
| ATON | 487 | H | THR | 49 | 46.138 | 8.041 | 67.673 | 1.00 | 38.95 | AAAA | N |
| ATON | 499 | CA | THR | 49 | 45.045 | 8.151 | 68.574 | 1.00 | 37.96 | AAAA | C |
| ATON | 490 | CB | THR | 49 | 45.548 | 8.207 | 70.034 | 1.00 | 48.69 | AAAA | C |
| ATON | 491 | CG1 | THR | 49 | 46.396 | 9.340 | 70.225 | 1.00 | 35.90 | AAAA | O |
| ATON | 493 | CG2 | THR | 49 | 46.230 | 6.957 | 70.529 | 1.00 | 31.99 | AAAA | C |
| ATON | 494 | C | THR | 49 | 44.230 | 9.425 | 68.321 | 1.00 | 39.48 | AAAA | C |
| ATON | 495 | O | THR | 49 | 43.111 | 9.451 | 68.837 | 1.00 | 34.49 | AAAA | O |
| ATON | 496 | H | VAL | 50 | 44.735 | 10.415 | 67.605 | 1.00 | 37.32 | AAAA | N |
| ATON | 499 | CA | VAL | 50 | 43.995 | 11.664 | 67.418 | 1.00 | 38.72 | AAAA | C |
| ATON | 499 | CB | VAL | 50 | 44.293 | 12.708 | 68.503 | 1.00 | 37.24 | AAAA | C |
| ATON | 500 | CG1 | VAL | 50 | 43.630 | 14.066 | 68.208 | 1.00 | 29.96 | AAAA | C |
| ATON | 501 | CG2 | VAL | 50 | 43.884 | 12.311 | 69.913 | 1.00 | 32.52 | AAAA | C |
| ATON | 502 | C | VAL | 50 | 44.271 | 12.305 | 66.048 | 1.00 | 37.03 | AAAA | C |
| ATON | 503 | O | VAL | 50 | 45.195 | 11.863 | 65.431 | 1.00 | 37.96 | AAAA | O |
| ATON | 504 | H | ILE | 51 | 43.319 | 12.939 | 65.415 | 1.00 | 37.49 | AAAA | N |
| ATON | 506 | CA | ILE | 51 | 43.301 | 13.575 | 64.133 | 1.00 | 32.48 | AAAA | C |
| ATON | 507 | CB | ILE | 51 | 42.346 | 12.864 | 63.152 | 1.00 | 34.51 | AAAA | C |
| ATON | 508 | CG2 | ILE | 51 | 41.995 | 13.802 | 61.978 | 1.00 | 32.31 | AAAA | C |
| ATON | 509 | CG1 | ILE | 51 | 43.026 | 11.611 | 62.671 | 1.00 | 30.78 | AAAA | C |
| ATON | 510 | CD1 | ILE | 51 | 42.358 | 10.559 | 61.815 | 1.00 | 19.69 | AAAA | C |
| ATON | 511 | C | ILE | 51 | 42.659 | 14.939 | 64.431 | 1.00 | 34.14 | AAAA | C |
| ATON | 512 | O | ILE | 51 | 41.546 | 14.830 | 64.923 | 1.00 | 29.08 | AAAA | O |
| ATON | 513 | H | THR | 52 | 43.342 | 16.058 | 64.238 | 1.00 | 33.93 | AAAA | N |
| ATON | 515 | CA | THR | 52 | 42.806 | 17.305 | 64.719 | 1.00 | 33.83 | AAAA | C |
| ATON | 516 | CB | THR | 52 | 43.961 | 18.338 | 64.939 | 1.00 | 35.39 | AAAA | C |
| ATON | 517 | CG1 | THR | 52 | 44.726 | 18.567 | 63.781 | 1.00 | 41.28 | AAAA | O |
| ATON | 519 | CG2 | THR | 52 | 44.775 | 17.926 | 66.134 | 1.00 | 22.01 | AAAA | C |
| ATON | 520 | C | THR | 52 | 41.741 | 17.961 | 63.863 | 1.00 | 39.02 | AAAA | C |
| ATON | 521 | O | THR | 52 | 41.202 | 19.030 | 64.243 | 1.00 | 38.88 | AAAA | O |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 522 | H | GLU | 53 | 41.524 | 17.477 | 62.639 | 1.00 | 36.93 | AAAA | N |
| ATOM | 524 | CA | GLU | 53 | 40.434 | 17.953 | 61.785 | 1.00 | 38.38 | AAAA | C |
| ATOM | 525 | CB | GLU | 53 | 41.064 | 18.512 | 60.483 | 1.00 | 29.76 | AAAA | C |
| ATOM | 526 | CG | GLU | 53 | 42.061 | 19.552 | 60.834 | 1.00 | 30.48 | AAAA | C |
| ATOM | 527 | CD | GLU | 53 | 42.517 | 20.396 | 59.697 | 1.00 | 40.82 | AAAA | C |
| ATOM | 528 | OE1 | GLU | 53 | 42.638 | 19.908 | 58.556 | 1.00 | 57.56 | AAAA | O |
| ATOM | 529 | OE2 | GLU | 53 | 42.799 | 21.559 | 59.931 | 1.00 | 35.74 | AAAA | O |
| ATOM | 530 | C | GLU | 53 | 39.506 | 16.789 | 61.388 | 1.00 | 39.19 | AAAA | C |
| ATOM | 531 | O | GLU | 53 | 38.922 | 16.311 | 62.386 | 1.00 | 38.95 | AAAA | O |
| ATOM | 532 | H | TYR | 54 | 39.639 | 16.353 | 60.102 | 1.00 | 30.60 | AAAA | N |
| ATOM | 534 | CA | TYR | 54 | 38.666 | 15.342 | 59.713 | 1.00 | 35.96 | AAAA | C |
| ATOM | 535 | CB | TYR | 54 | 37.654 | 15.602 | 58.636 | 1.00 | 30.71 | AAAA | C |
| ATOM | 536 | CG | TYR | 54 | 38.247 | 16.476 | 57.388 | 1.00 | 21.18 | AAAA | C |
| ATOM | 537 | CD1 | TYR | 54 | 38.487 | 15.733 | 56.305 | 1.00 | 20.22 | AAAA | C |
| ATOM | 538 | CE1 | TYR | 54 | 38.980 | 16.243 | 55.086 | 1.00 | 21.04 | AAAA | C |
| ATOM | 539 | CD2 | TYR | 54 | 38.577 | 17.944 | 57.307 | 1.00 | 23.97 | AAAA | C |
| ATOM | 540 | CE2 | TYR | 54 | 39.049 | 18.394 | 56.124 | 1.00 | 24.69 | AAAA | C |
| ATOM | 541 | CZ | TYR | 54 | 39.263 | 17.569 | 55.032 | 1.00 | 26.72 | AAAA | C |
| ATOM | 542 | OH | TYR | 54 | 39.763 | 18.047 | 53.847 | 1.00 | 37.55 | AAAA | O |
| ATOM | 544 | C | TYR | 54 | 39.405 | 14.115 | 59.142 | 1.00 | 33.87 | AAAA | C |
| ATOM | 545 | O | TYR | 54 | 40.513 | 14.360 | 58.678 | 1.00 | 30.40 | AAAA | O |
| ATOM | 546 | H | LEU | 55 | 38.683 | 13.021 | 59.004 | 1.00 | 23.24 | AAAA | H |
| ATOM | 548 | CA | LEU | 55 | 39.111 | 11.812 | 58.454 | 1.00 | 30.08 | AAAA | C |
| ATOM | 549 | CB | LEU | 55 | 39.011 | 10.663 | 59.510 | 1.00 | 14.78 | AAAA | C |
| ATOM | 550 | CG | LEU | 55 | 39.349 | 9.314 | 58.818 | 1.00 | 26.98 | AAAA | C |
| ATOM | 551 | CD1 | LEU | 55 | 40.668 | 9.477 | 58.040 | 1.00 | 26.66 | AAAA | C |
| ATOM | 552 | CD2 | LEU | 55 | 39.496 | 8.093 | 59.705 | 1.00 | 14.45 | AAAA | C |
| ATOM | 553 | C | LEU | 55 | 38.201 | 11.548 | 57.238 | 1.00 | 37.43 | AAAA | C |
| ATOM | 554 | O | LEU | 55 | 36.995 | 11.632 | 57.427 | 1.00 | 39.55 | AAAA | O |
| ATOM | 555 | H | LEU | 56 | 38.700 | 11.348 | 56.035 | 1.00 | 41.83 | AAAA | N |
| ATOM | 557 | CA | LEU | 56 | 37.955 | 11.201 | 54.799 | 1.00 | 36.98 | AAAA | C |
| ATOM | 558 | CB | LEU | 56 | 37.998 | 12.446 | 53.949 | 1.00 | 33.29 | AAAA | C |
| ATOM | 559 | CG | LEU | 56 | 37.984 | 12.514 | 52.416 | 1.00 | 30.35 | AAAA | C |
| ATOM | 560 | CD1 | LEU | 56 | 37.076 | 11.460 | 51.821 | 1.00 | 47.95 | AAAA | C |
| ATOM | 561 | CD2 | LEU | 56 | 37.286 | 13.807 | 51.985 | 1.00 | 33.47 | AAAA | C |
| ATOM | 562 | C | LEU | 56 | 38.595 | 10.047 | 54.008 | 1.00 | 39.75 | AAAA | C |
| ATOM | 563 | O | LEU | 56 | 39.714 | 10.205 | 53.547 | 1.00 | 44.38 | AAAA | O |
| ATOM | 564 | H | LEU | 57 | 37.846 | 9.008 | 53.800 | 1.00 | 36.68 | AAAA | H |
| ATOM | 566 | CA | LEU | 57 | 38.133 | 7.810 | 53.034 | 1.00 | 41.53 | AAAA | C |
| ATOM | 567 | CB | LEU | 57 | 37.944 | 6.598 | 53.916 | 1.00 | 37.00 | AAAA | C |
| ATOM | 568 | CG | LEU | 57 | 39.064 | 6.534 | 55.026 | 1.00 | 36.13 | AAAA | C |
| ATOM | 569 | CD1 | LEU | 57 | 38.513 | 6.990 | 56.417 | 1.00 | 33.26 | AAAA | C |
| ATOM | 570 | CD2 | LEU | 57 | 39.630 | 5.160 | 55.039 | 1.00 | 24.11 | AAAA | C |
| ATOM | 571 | C | LEU | 57 | 37.203 | 7.815 | 51.838 | 1.00 | 46.03 | AAAA | C |
| ATOM | 572 | O | LEU | 57 | 35.985 | 7.993 | 51.969 | 1.00 | 44.78 | AAAA | O |
| ATOM | 573 | H | PHE | 58 | 37.792 | 7.998 | 50.642 | 1.00 | 47.07 | AAAA | H |
| ATOM | 575 | CA | PHE | 58 | 36.995 | 9.102 | 49.467 | 1.00 | 49.75 | AAAA | C |
| ATOM | 576 | CB | PHE | 58 | 36.704 | 9.448 | 49.102 | 1.00 | 46.67 | AAAA | C |
| ATOM | 577 | CG | PHE | 58 | 36.447 | 9.818 | 47.692 | 1.00 | 54.66 | AAAA | C |
| ATOM | 578 | CD1 | PHE | 58 | 37.413 | 9.706 | 46.697 | 1.00 | 55.19 | AAAA | C |
| ATOM | 579 | CD2 | PHE | 58 | 35.209 | 10.311 | 47.326 | 1.00 | 53.96 | AAAA | C |
| ATOM | 580 | CE1 | PHE | 58 | 37.124 | 10.763 | 45.396 | 1.00 | 50.36 | AAAA | C |
| ATOM | 581 | CE2 | PHE | 58 | 34.985 | 10.655 | 46.011 | 1.00 | 41.84 | AAAA | C |
| ATOM | 582 | CZ | PHE | 58 | 35.877 | 10.501 | 45.037 | 1.00 | 46.50 | AAAA | C |
| ATOM | 583 | O | PHE | 58 | 37.351 | 7.052 | 48.379 | 1.00 | 49.71 | AAAA | C |
| ATOM | 584 | C | PHE | 58 | 38.487 | 7.073 | 47.934 | 1.00 | 52.16 | AAAA | O |
| ATOM | 585 | H | ARG | 59 | 36.471 | 6.118 | 47.944 | 1.00 | 44.26 | AAAA | N |
| ATOM | 587 | CA | ARG | 59 | 36.753 | 5.281 | 46.815 | 1.00 | 40.80 | AAAA | C |
| ATOM | 588 | CB | ARG | 59 | 36.911 | 5.993 | 45.427 | 1.00 | 23.79 | AAAA | C |
| ATOM | 589 | CG | ARG | 59 | 35.869 | 7.020 | 45.121 | 1.00 | 46.53 | AAAA | C |
| ATOM | 590 | CD | ARG | 59 | 35.921 | 7.562 | 43.706 | 1.00 | 37.64 | AAAA | C |
| ATOM | 591 | NE | ARG | 59 | 35.822 | 6.422 | 42.806 | 1.00 | 49.23 | AAAA | N |
| ATOM | 593 | CZ | ARG | 59 | 34.950 | 5.932 | 42.036 | 1.00 | 41.36 | AAAA | C |
| ATOM | 594 | HH1 | ARG | 59 | 33.702 | 6.277 | 41.931 | 1.00 | 47.00 | AAAA | N |
| ATOM | 597 | HH2 | ARG | 59 | 35.237 | 4.729 | 41.327 | 1.00 | 42.58 | AAAA | H |
| ATOM | 600 | C | ARG | 59 | 38.037 | 4.494 | 47.049 | 1.00 | 42.25 | AAAA | C |
| ATOM | 601 | O | ARG | 59 | 38.981 | 4.513 | 46.232 | 1.00 | 44.11 | AAAA | O |
| ATOM | 602 | H | VAL | 60 | 38.001 | 3.625 | 48.023 | 1.00 | 40.94 | AAAA | H |
| ATOM | 604 | CA | VAL | 60 | 39.101 | 2.743 | 48.341 | 1.00 | 39.14 | AAAA | C |
| ATOM | 605 | CB | VAL | 60 | 39.624 | 3.066 | 49.751 | 1.00 | 40.12 | AAAA | C |
| ATOM | 606 | CG1 | VAL | 60 | 40.407 | 1.872 | 50.296 | 1.00 | 35.05 | AAAA | C |
| ATOM | 607 | CG2 | VAL | 60 | 40.425 | 4.352 | 49.893 | 1.00 | 28.86 | AAAA | C |
| ATOM | 608 | C | VAL | 60 | 38.539 | 1.337 | 48.368 | 1.00 | 43.56 | AAAA | C |
| ATOM | 609 | O | VAL | 60 | 37.535 | 1.224 | 49.072 | 1.00 | 47.66 | AAAA | O |
| ATOM | 610 | H | ALA | 61 | 39.094 | 0.371 | 47.659 | 1.00 | 41.92 | AAAA | H |
| ATOM | 612 | CA | ALA | 61 | 38.617 | -0.992 | 47.749 | 1.00 | 42.05 | AAAA | C |
| ATOM | 613 | CB | ALA | 61 | 38.302 | -1.483 | 46.364 | 1.00 | 52.40 | AAAA | C |
| ATOM | 614 | C | ALA | 61 | 39.613 | -1.934 | 48.386 | 1.00 | 43.08 | AAAA | C |
| ATOM | 615 | O | ALA | 61 | 40.757 | -1.602 | 48.670 | 1.00 | 50.59 | AAAA | O |
| ATOM | 616 | H | GLY | 62 | 39.200 | -3.105 | 48.849 | 1.00 | 45.71 | AAAA | H |
| ATOM | 618 | CA | GLY | 62 | 40.136 | -4.079 | 49.385 | 1.00 | 45.39 | AAAA | C |
| ATOM | 619 | C | GLY | 62 | 40.262 | -3.902 | 50.872 | 1.00 | 48.04 | AAAA | C |
| ATOM | 620 | O | GLY | 62 | 40.587 | -4.835 | 51.604 | 1.00 | 52.34 | AAAA | O |
| ATOM | 621 | H | LEU | 63 | 39.985 | -2.734 | 51.383 | 1.00 | 46.90 | AAAA | H |
| ATOM | 623 | CA | LEU | 63 | 40.003 | -2.443 | 52.805 | 1.00 | 49.11 | AAAA | C |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 624 | CB | LEU | 63 | 40.274 | -0.953 | 53.027 | 1.00 | 41.41 | AAAA | C |
| ATOM | 625 | CG | LEU | 63 | 40.265 | -0.423 | 54.443 | 1.00 | 53.41 | AAAA | C |
| ATOM | 626 | CD1 | LEU | 63 | 41.172 | -1.164 | 55.416 | 1.00 | 48.27 | AAAA | C |
| ATOM | 627 | CD2 | LEU | 63 | 40.637 | 1.047 | 54.246 | 1.00 | 50.51 | AAAA | C |
| ATOM | 628 | C | LEU | 63 | 38.643 | -2.881 | 53.323 | 1.00 | 54.20 | AAAA | C |
| ATOM | 629 | O | LEU | 63 | 37.587 | -2.430 | 52.837 | 1.00 | 57.73 | AAAA | O |
| ATOM | 630 | H | GLU | 64 | 38.658 | -3.862 | 54.190 | 1.00 | 53.97 | AAAA | H |
| ATOM | 632 | CA | GLU | 64 | 37.462 | -4.448 | 54.749 | 1.00 | 56.96 | AAAA | C |
| ATOM | 633 | CB | GLU | 64 | 37.689 | -5.956 | 54.734 | 1.00 | 65.33 | AAAA | C |
| ATOM | 634 | CG | GLU | 64 | 37.832 | -6.484 | 53.293 | 1.00 | 75.14 | AAAA | C |
| ATOM | 635 | CD | GLU | 64 | 37.404 | -7.940 | 53.128 | 1.00 | 78.10 | AAAA | C |
| ATOM | 636 | OE1 | GLU | 64 | 37.424 | -8.698 | 54.132 | 1.00 | 63.93 | AAAA | O |
| ATOM | 637 | OE2 | GLU | 64 | 37.036 | -8.320 | 51.978 | 1.00 | 88.77 | AAAA | O |
| ATOM | 638 | C | GLU | 64 | 37.096 | -4.007 | 56.163 | 1.00 | 57.12 | AAAA | C |
| ATOM | 639 | O | GLU | 64 | 35.986 | -4.332 | 56.600 | 1.00 | 59.82 | AAAA | O |
| ATOM | 640 | H | SER | 65 | 37.766 | -3.042 | 56.761 | 1.00 | 50.64 | AAAA | H |
| ATOM | 642 | CA | SER | 65 | 37.539 | -2.523 | 58.060 | 1.00 | 47.19 | AAAA | C |
| ATOM | 643 | CB | SER | 65 | 37.743 | -3.596 | 59.139 | 1.00 | 49.24 | AAAA | C |
| ATOM | 644 | CG | SER | 65 | 37.501 | -2.971 | 60.429 | 1.00 | 50.90 | AAAA | O |
| ATOM | 646 | C | SER | 65 | 38.516 | -1.405 | 58.432 | 1.00 | 48.35 | AAAA | C |
| ATOM | 647 | O | SER | 65 | 39.716 | -1.692 | 58.374 | 1.00 | 52.75 | AAAA | O |
| ATOM | 648 | H | LEU | 66 | 38.054 | -0.289 | 58.984 | 1.00 | 41.03 | AAAA | H |
| ATOM | 650 | CA | LEU | 66 | 38.956 | 0.758 | 59.405 | 1.00 | 41.94 | AAAA | C |
| ATOM | 651 | CB | LEU | 66 | 38.247 | 2.083 | 59.498 | 1.00 | 25.25 | AAAA | C |
| ATOM | 652 | CG | LEU | 66 | 37.283 | 2.476 | 58.402 | 1.00 | 34.49 | AAAA | C |
| ATOM | 653 | CD1 | LEU | 66 | 36.974 | 3.951 | 58.512 | 1.00 | 30.81 | AAAA | C |
| ATOM | 654 | CD2 | LEU | 66 | 37.767 | 2.200 | 56.994 | 1.00 | 34.34 | AAAA | C |
| ATOM | 655 | C | LEU | 66 | 39.646 | 0.462 | 60.734 | 1.00 | 45.39 | AAAA | C |
| ATOM | 656 | O | LEU | 66 | 40.762 | 0.947 | 60.927 | 1.00 | 41.05 | AAAA | O |
| ATOM | 657 | N | GLY | 67 | 39.000 | -0.346 | 61.583 | 1.00 | 45.21 | AAAA | N |
| ATOM | 659 | CA | GLY | 67 | 39.773 | -0.672 | 62.799 | 1.00 | 48.14 | AAAA | C |
| ATOM | 660 | C | GLY | 67 | 40.998 | -1.508 | 62.445 | 1.00 | 44.51 | AAAA | C |
| ATOM | 661 | O | GLY | 67 | 41.855 | -1.724 | 63.287 | 1.00 | 45.42 | AAAA | O |
| ATOM | 662 | H | ASP | 68 | 41.013 | -2.189 | 61.309 | 1.00 | 47.60 | AAAA | H |
| ATOM | 664 | CA | ASP | 68 | 42.194 | -2.834 | 60.738 | 1.00 | 50.99 | AAAA | C |
| ATOM | 665 | CB | ASP | 68 | 42.012 | -3.417 | 59.361 | 1.00 | 39.43 | AAAA | C |
| ATOM | 666 | CG | ASP | 68 | 41.205 | -4.679 | 59.311 | 1.00 | 45.82 | AAAA | C |
| ATOM | 667 | CD1 | ASP | 68 | 40.912 | -5.341 | 60.320 | 1.00 | 44.69 | AAAA | O |
| ATOM | 668 | CD2 | ASP | 68 | 40.819 | -5.065 | 58.187 | 1.00 | 47.23 | AAAA | O |
| ATOM | 669 | C | ASP | 68 | 43.363 | -1.837 | 60.596 | 1.00 | 45.89 | AAAA | C |
| ATOM | 670 | O | ASP | 68 | 44.436 | -2.269 | 60.903 | 1.00 | 44.84 | AAAA | O |
| ATOM | 671 | H | LEU | 69 | 43.145 | -0.609 | 60.247 | 1.00 | 42.49 | AAAA | H |
| ATOM | 673 | CA | LEU | 69 | 44.175 | 0.352 | 60.049 | 1.00 | 45.90 | AAAA | C |
| ATOM | 674 | CB | LEU | 69 | 43.920 | 1.393 | 58.945 | 1.00 | 45.25 | AAAA | C |
| ATOM | 675 | CG | LEU | 69 | 43.902 | 0.882 | 57.494 | 1.00 | 54.25 | AAAA | C |
| ATOM | 676 | CD1 | LEU | 69 | 43.541 | 2.037 | 56.565 | 1.00 | 47.26 | AAAA | C |
| ATOM | 677 | CD2 | LEU | 69 | 45.211 | 0.200 | 57.113 | 1.00 | 50.76 | AAAA | C |
| ATOM | 678 | C | LEU | 69 | 44.347 | 1.107 | 61.350 | 1.00 | 49.50 | AAAA | C |
| ATOM | 679 | O | LEU | 69 | 45.470 | 1.210 | 61.851 | 1.00 | 54.51 | AAAA | O |
| ATOM | 680 | H | PHE | 70 | 43.296 | 1.737 | 61.869 | 1.00 | 44.60 | AAAA | H |
| ATOM | 682 | CA | PHE | 70 | 43.423 | 2.564 | 63.046 | 1.00 | 39.67 | AAAA | C |
| ATOM | 683 | CB | PHE | 70 | 42.997 | 3.973 | 62.700 | 1.00 | 26.08 | AAAA | C |
| ATOM | 684 | CG | PHE | 70 | 43.465 | 4.501 | 61.390 | 1.00 | 45.32 | AAAA | C |
| ATOM | 685 | CD1 | PHE | 70 | 42.532 | 4.749 | 60.384 | 1.00 | 47.41 | AAAA | C |
| ATOM | 686 | CD2 | PHE | 70 | 44.815 | 4.767 | 61.130 | 1.00 | 48.77 | AAAA | C |
| ATOM | 687 | CE1 | PHE | 70 | 42.945 | 5.263 | 59.159 | 1.00 | 56.16 | AAAA | C |
| ATOM | 688 | CE2 | PHE | 70 | 45.229 | 5.256 | 59.895 | 1.00 | 47.24 | AAAA | C |
| ATOM | 689 | CC | PHE | 70 | 44.293 | 5.506 | 58.896 | 1.00 | 49.54 | AAAA | C |
| ATOM | 690 | C | PHE | 70 | 42.655 | 1.999 | 64.219 | 1.00 | 40.09 | AAAA | C |
| ATOM | 691 | O | PHE | 70 | 41.874 | 2.734 | 64.838 | 1.00 | 35.74 | AAAA | O |
| ATOM | 692 | H | PRO | 71 | 43.053 | 0.852 | 64.768 | 1.00 | 39.19 | AAAA | N |
| ATOM | 693 | CD | PRO | 71 | 44.269 | 0.058 | 64.411 | 1.00 | 39.94 | AAAA | C |
| ATOM | 694 | CA | PRO | 71 | 42.444 | 0.237 | 65.899 | 1.00 | 35.30 | AAAA | C |
| ATOM | 695 | CB | PRO | 71 | 43.308 | -0.983 | 66.246 | 1.00 | 38.03 | AAAA | C |
| ATOM | 696 | CG | PRO | 71 | 44.669 | -0.564 | 65.717 | 1.00 | 38.36 | AAAA | C |
| ATOM | 697 | C | PRO | 71 | 42.453 | 1.089 | 67.126 | 1.00 | 33.72 | AAAA | C |
| ATOM | 698 | O | PRO | 71 | 42.005 | 0.630 | 68.159 | 1.00 | 39.32 | AAAA | O |
| ATOM | 699 | N | ASN | 72 | 43.058 | 2.220 | 67.231 | 1.00 | 36.55 | AAAA | H |
| ATOM | 701 | CA | ASN | 72 | 43.204 | 3.032 | 68.401 | 1.00 | 32.60 | AAAA | C |
| ATOM | 702 | CB | ASN | 72 | 44.637 | 2.916 | 68.962 | 1.00 | 36.89 | AAAA | C |
| ATOM | 703 | CG | ASN | 72 | 44.735 | 1.638 | 69.761 | 1.00 | 47.03 | AAAA | C |
| ATOM | 704 | CD1 | ASN | 72 | 44.644 | 1.619 | 70.979 | 1.00 | 64.42 | AAAA | O |
| ATOM | 705 | HD2 | ASN | 72 | 44.880 | 0.475 | 69.169 | 1.00 | 63.17 | AAAA | H |
| ATOM | 708 | C | ASN | 72 | 42.875 | 4.477 | 68.135 | 1.00 | 30.11 | AAAA | C |
| ATOM | 709 | O | ASN | 72 | 43.099 | 5.201 | 69.104 | 1.00 | 36.53 | AAAA | O |
| ATOM | 710 | H | LEU | 73 | 42.309 | 4.809 | 66.978 | 1.00 | 27.62 | AAAA | H |
| ATOM | 712 | CA | LEU | 73 | 41.940 | 6.207 | 66.730 | 1.00 | 34.07 | AAAA | C |
| ATOM | 713 | CB | LEU | 73 | 41.476 | 6.373 | 65.292 | 1.00 | 28.37 | AAAA | C |
| ATOM | 714 | CG | LEU | 73 | 40.819 | 7.713 | 64.882 | 1.00 | 29.33 | AAAA | C |
| ATOM | 715 | CD1 | LEU | 73 | 41.918 | 8.721 | 64.963 | 1.00 | 31.86 | AAAA | C |
| ATOM | 716 | CD2 | LEU | 73 | 40.202 | 7.518 | 63.478 | 1.00 | 32.07 | AAAA | C |
| ATOM | 717 | C | LEU | 73 | 40.929 | 6.569 | 67.817 | 1.00 | 32.14 | AAAA | C |
| ATOM | 718 | O | LEU | 73 | 40.073 | 5.737 | 68.081 | 1.00 | 35.02 | AAAA | O |
| ATOM | 719 | H | THR | 74 | 41.081 | 7.585 | 68.582 | 1.00 | 29.47 | AAAA | H |
| ATOM | 721 | CA | THR | 74 | 40.150 | 7.826 | 69.683 | 1.00 | 34.80 | AAAA | C |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 700 | CB | THR | 74 | 41.028 | 7.744 | 70.952 | 1.00 | 46.09 | AAAA | C |
| ATOM | 703 | CG1 | THR | 74 | 41.729 | 6.485 | 70.880 | 1.00 | 46.30 | AAAA | O |
| ATOM | 725 | CG2 | THR | 74 | 40.262 | 7.831 | 72.253 | 1.00 | 39.45 | AAAA | C |
| ATOM | 726 | C | THR | 74 | 39.424 | 9.155 | 69.602 | 1.00 | 35.48 | AAAA | C |
| ATOM | 727 | O | THR | 74 | 38.270 | 9.322 | 70.077 | 1.00 | 35.32 | AAAA | O |
| ATOM | 728 | H | VAL | 75 | 40.047 | 10.198 | 69.073 | 1.00 | 29.80 | AAAA | H |
| ATOM | 730 | CA | VAL | 75 | 39.351 | 11.474 | 68.892 | 1.00 | 34.91 | AAAA | C |
| ATOM | 731 | CB | VAL | 75 | 39.856 | 12.445 | 69.955 | 1.00 | 26.03 | AAAA | C |
| ATOM | 732 | CG1 | VAL | 75 | 39.173 | 13.801 | 69.934 | 1.00 | 24.51 | AAAA | C |
| ATOM | 733 | CG2 | VAL | 75 | 39.675 | 11.910 | 71.366 | 1.00 | 19.87 | AAAA | C |
| ATOM | 734 | C | VAL | 75 | 39.613 | 12.045 | 67.494 | 1.00 | 37.57 | AAAA | C |
| ATOM | 735 | O | VAL | 75 | 40.724 | 11.808 | 67.022 | 1.00 | 35.99 | AAAA | O |
| ATOM | 736 | H | ILE | 76 | 38.600 | 12.555 | 66.796 | 1.00 | 35.91 | AAAA | H |
| ATOM | 738 | CA | ILE | 76 | 38.696 | 13.340 | 65.592 | 1.00 | 31.48 | AAAA | C |
| ATOM | 739 | CB | ILE | 76 | 37.831 | 12.769 | 64.492 | 1.00 | 29.60 | AAAA | C |
| ATOM | 740 | CG2 | ILE | 76 | 37.856 | 13.630 | 63.208 | 1.00 | 19.54 | AAAA | C |
| ATOM | 741 | CG1 | ILE | 76 | 38.222 | 11.314 | 64.277 | 1.00 | 28.52 | AAAA | C |
| ATOM | 742 | CD1 | ILE | 76 | 37.149 | 10.556 | 63.478 | 1.00 | 28.85 | AAAA | C |
| ATOM | 743 | C | ILE | 76 | 38.157 | 14.718 | 66.000 | 1.00 | 33.84 | AAAA | C |
| ATOM | 744 | O | ILE | 76 | 36.987 | 14.777 | 66.274 | 1.00 | 38.84 | AAAA | O |
| ATOM | 745 | H | ARG | 77 | 38.906 | 15.733 | 66.230 | 1.00 | 30.32 | AAAA | H |
| ATOM | 747 | CA | ARG | 77 | 38.605 | 16.901 | 67.021 | 1.00 | 30.82 | AAAA | C |
| ATOM | 748 | CB | ARG | 77 | 39.961 | 17.475 | 67.461 | 1.00 | 26.62 | AAAA | C |
| ATOM | 749 | CG | ARG | 77 | 39.993 | 18.836 | 68.058 | 1.00 | 52.42 | AAAA | C |
| ATOM | 750 | CD | ARG | 77 | 41.290 | 18.957 | 68.908 | 1.00 | 49.10 | AAAA | C |
| ATOM | 751 | HE | ARG | 77 | 41.411 | 17.817 | 69.773 | 1.00 | 39.23 | AAAA | H |
| ATOM | 753 | CE | ARG | 77 | 40.977 | 18.016 | 71.064 | 1.00 | 48.79 | AAAA | C |
| ATOM | 754 | NH1 | ARG | 77 | 40.440 | 19.104 | 71.610 | 1.00 | 30.34 | AAAA | H |
| ATOM | 757 | NH2 | ARG | 77 | 41.061 | 17.012 | 71.941 | 1.00 | 40.38 | AAAA | N |
| ATOM | 760 | C | ARG | 77 | 37.643 | 17.733 | 66.225 | 1.00 | 31.75 | AAAA | C |
| ATOM | 761 | O | ARG | 77 | 36.944 | 18.637 | 66.664 | 1.00 | 31.40 | AAAA | O |
| ATOM | 762 | H | GLY | 78 | 37.688 | 17.661 | 64.884 | 1.00 | 32.87 | AAAA | H |
| ATOM | 764 | CA | GLY | 78 | 36.982 | 18.409 | 63.950 | 1.00 | 16.23 | AAAA | C |
| ATOM | 765 | C | GLY | 78 | 37.199 | 19.880 | 64.063 | 1.00 | 31.58 | AAAA | C |
| ATOM | 766 | O | GLY | 78 | 36.363 | 20.775 | 63.674 | 1.00 | 34.03 | AAAA | O |
| ATOM | 767 | H | TRP | 79 | 38.439 | 20.321 | 64.304 | 1.00 | 31.21 | AAAA | H |
| ATOM | 769 | CA | TRP | 79 | 38.757 | 21.740 | 64.337 | 1.00 | 30.80 | AAAA | C |
| ATOM | 770 | CB | TRP | 79 | 40.177 | 21.943 | 64.845 | 1.00 | 39.07 | AAAA | C |
| ATOM | 771 | CG | TRP | 79 | 40.626 | 23.343 | 65.164 | 1.00 | 36.64 | AAAA | C |
| ATOM | 772 | CD2 | TRP | 79 | 41.691 | 24.001 | 64.433 | 1.00 | 28.52 | AAAA | C |
| ATOM | 773 | CE2 | TRP | 79 | 41.826 | 25.288 | 65.002 | 1.00 | 36.49 | AAAA | C |
| ATOM | 774 | CE3 | TRP | 79 | 42.473 | 23.625 | 63.370 | 1.00 | 37.96 | AAAA | C |
| ATOM | 775 | CD1 | TRP | 79 | 40.199 | 24.235 | 66.113 | 1.00 | 29.59 | AAAA | C |
| ATOM | 776 | NH1 | TRP | 79 | 40.917 | 25.413 | 66.054 | 1.00 | 27.67 | AAAA | H |
| ATOM | 778 | CD2 | TRP | 79 | 42.770 | 26.213 | 64.543 | 1.00 | 31.83 | AAAA | C |
| ATOM | 779 | CD3 | TRP | 79 | 43.389 | 24.548 | 62.876 | 1.00 | 46.14 | AAAA | C |
| ATOM | 780 | CH2 | TRP | 79 | 43.525 | 25.794 | 63.470 | 1.00 | 35.31 | AAAA | C |
| ATOM | 781 | C | TRP | 79 | 38.606 | 23.418 | 62.986 | 1.00 | 28.75 | AAAA | C |
| ATOM | 782 | O | TRP | 79 | 38.585 | 23.624 | 62.961 | 1.00 | 23.61 | AAAA | O |
| ATOM | 783 | H | LYS | 80 | 38.659 | 21.694 | 61.895 | 1.00 | 31.84 | AAAA | H |
| ATOM | 785 | CA | LYS | 80 | 38.305 | 22.153 | 60.573 | 1.00 | 32.72 | AAAA | C |
| ATOM | 786 | CB | LYS | 80 | 39.453 | 22.498 | 59.689 | 1.00 | 41.17 | AAAA | C |
| ATOM | 787 | CG | LYS | 80 | 39.938 | 23.911 | 59.470 | 1.00 | 34.69 | AAAA | C |
| ATOM | 788 | CD | LYS | 80 | 41.025 | 24.350 | 60.306 | 1.00 | 44.77 | AAAA | C |
| ATOM | 789 | CE | LYS | 80 | 41.276 | 25.811 | 59.898 | 1.00 | 50.41 | AAAA | C |
| ATOM | 790 | NZ | LYS | 80 | 42.530 | 25.752 | 59.092 | 1.00 | 67.26 | AAAA | H |
| ATOM | 791 | C | LYS | 80 | 37.585 | 20.960 | 59.917 | 1.00 | 34.52 | AAAA | C |
| ATOM | 792 | O | LYS | 80 | 37.950 | 19.843 | 60.237 | 1.00 | 37.62 | AAAA | O |
| ATOM | 793 | H | LEU | 81 | 36.477 | 21.267 | 59.207 | 1.00 | 31.77 | AAAA | H |
| ATOM | 795 | CA | LEU | 81 | 35.742 | 20.157 | 58.600 | 1.00 | 31.02 | AAAA | C |
| ATOM | 796 | CB | LEU | 81 | 34.290 | 20.315 | 59.092 | 1.00 | 31.20 | AAAA | C |
| ATOM | 797 | CG | LEU | 81 | 34.115 | 20.319 | 60.632 | 1.00 | 36.97 | AAAA | C |
| ATOM | 798 | CD1 | LEU | 81 | 32.832 | 21.080 | 60.954 | 1.00 | 27.98 | AAAA | C |
| ATOM | 799 | CD2 | LEU | 81 | 34.089 | 18.955 | 61.297 | 1.00 | 28.77 | AAAA | C |
| ATOM | 800 | C | LEU | 81 | 35.733 | 20.023 | 57.104 | 1.00 | 29.86 | AAAA | C |
| ATOM | 801 | O | LEU | 81 | 36.082 | 20.947 | 56.368 | 1.00 | 29.34 | AAAA | O |
| ATOM | 802 | H | PHE | 82 | 35.430 | 18.813 | 56.594 | 1.00 | 27.78 | AAAA | H |
| ATOM | 804 | CA | PHE | 82 | 35.176 | 19.653 | 55.182 | 1.00 | 28.68 | AAAA | C |
| ATOM | 805 | CB | PHE | 82 | 35.513 | 17.226 | 54.795 | 1.00 | 32.78 | AAAA | C |
| ATOM | 806 | CG | PHE | 82 | 35.348 | 16.901 | 53.357 | 1.00 | 30.48 | AAAA | C |
| ATOM | 807 | CD1 | PHE | 82 | 36.378 | 17.130 | 52.447 | 1.00 | 32.86 | AAAA | C |
| ATOM | 808 | CD2 | PHE | 82 | 34.142 | 16.361 | 52.914 | 1.00 | 30.93 | AAAA | C |
| ATOM | 809 | CE1 | PHE | 82 | 36.217 | 16.769 | 51.104 | 1.00 | 43.27 | AAAA | C |
| ATOM | 810 | CE2 | PHE | 82 | 33.963 | 16.061 | 51.538 | 1.00 | 26.30 | AAAA | C |
| ATOM | 811 | CE | PHE | 82 | 35.005 | 16.238 | 50.672 | 1.00 | 37.73 | AAAA | C |
| ATOM | 812 | C | PHE | 82 | 33.670 | 18.911 | 54.993 | 1.00 | 30.06 | AAAA | C |
| ATOM | 813 | O | PHE | 82 | 32.830 | 18.045 | 55.278 | 1.00 | 27.36 | AAAA | O |
| ATOM | 814 | H | TYR | 83 | 33.301 | 20.148 | 54.770 | 1.00 | 31.68 | AAAA | H |
| ATOM | 815 | CA | TYR | 83 | 31.911 | 20.605 | 54.633 | 1.00 | 40.76 | AAAA | C |
| ATOM | 816 | C | TYR | 83 | 31.043 | 19.977 | 55.726 | 1.00 | 44.00 | AAAA | C |
| ATOM | 817 | O | TYR | 83 | 30.075 | 19.210 | 55.487 | 1.00 | 50.47 | AAAA | O |
| ATOM | 818 | CB | TYR | 83 | 31.359 | 20.199 | 53.269 | 1.00 | 31.55 | AAAA | C |
| ATOM | 819 | CG | TYR | 83 | 32.196 | 20.742 | 52.117 | 0.01 | 20.00 | AAAA | C |
| ATOM | 820 | CD1 | TYR | 83 | 33.254 | 19.982 | 51.609 | 0.01 | 20.00 | AAAA | C |
| ATOM | 821 | CD2 | TYR | 83 | 31.906 | 21.998 | 51.575 | 0.01 | 20.00 | AAAA | C |

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|------|-----|-----|-----|----|--------|--------|--------|------|-------|------|---|
| ATOM | 802 | CE1 | TYR | 83 | 34.927 | 20.489 | 50.556 | 0.01 | 20.00 | AAAA | C |
| ATOM | 803 | CE2 | TYR | 83 | 32.679 | 22.496 | 50.521 | 0.01 | 20.00 | AAAA | C |
| ATOM | 804 | CE | TYR | 83 | 33.740 | 21.737 | 50.012 | 0.01 | 20.00 | AAAA | C |
| ATOM | 805 | OH | TYR | 83 | 34.492 | 22.222 | 48.989 | 0.01 | 20.00 | AAAA | O |
| ATOM | 806 | H | ASH | 84 | 31.043 | 20.461 | 56.924 | 1.00 | 40.91 | AAAA | N |
| ATOM | 807 | CA | ASH | 84 | 30.250 | 20.057 | 58.056 | 1.00 | 36.54 | AAAA | C |
| ATOM | 808 | CB | ASH | 84 | 28.763 | 20.046 | 57.700 | 1.00 | 47.84 | AAAA | C |
| ATOM | 809 | CG | ASH | 84 | 28.274 | 21.164 | 56.797 | 1.00 | 60.75 | AAAA | C |
| ATOM | 830 | OD1 | ASH | 84 | 28.319 | 22.343 | 57.119 | 1.00 | 45.55 | AAAA | O |
| ATOM | 831 | HD2 | ASH | 84 | 27.839 | 20.876 | 55.552 | 1.00 | 65.98 | AAAA | N |
| ATOM | 832 | C | ASH | 84 | 30.686 | 18.679 | 58.556 | 1.00 | 36.33 | AAAA | C |
| ATOM | 833 | O | ASH | 84 | 30.137 | 18.206 | 59.580 | 1.00 | 38.24 | AAAA | O |
| ATOM | 834 | H | TYR | 85 | 31.455 | 17.900 | 57.800 | 1.00 | 32.78 | AAAA | N |
| ATOM | 836 | CA | TYR | 85 | 31.617 | 16.504 | 58.222 | 1.00 | 35.45 | AAAA | C |
| ATOM | 837 | CB | TYR | 85 | 31.473 | 15.579 | 57.000 | 1.00 | 35.54 | AAAA | C |
| ATOM | 838 | CG | TYR | 85 | 30.078 | 15.733 | 56.453 | 1.00 | 41.35 | AAAA | C |
| ATOM | 839 | CD1 | TYR | 85 | 29.868 | 16.291 | 55.199 | 1.00 | 38.22 | AAAA | C |
| ATOM | 840 | CE1 | TYR | 85 | 28.611 | 16.445 | 54.704 | 1.00 | 40.83 | AAAA | C |
| ATOM | 841 | CD2 | TYR | 85 | 28.954 | 15.371 | 57.200 | 1.00 | 47.42 | AAAA | C |
| ATOM | 842 | CE2 | TYR | 85 | 27.661 | 15.533 | 56.705 | 1.00 | 45.91 | AAAA | C |
| ATOM | 843 | CS | TYR | 85 | 27.497 | 16.072 | 55.445 | 1.00 | 46.06 | AAAA | C |
| ATOM | 844 | OH | TYR | 85 | 26.258 | 16.315 | 54.886 | 1.00 | 46.05 | AAAA | O |
| ATOM | 846 | C | TYR | 85 | 32.977 | 16.367 | 58.891 | 1.00 | 32.08 | AAAA | C |
| ATOM | 847 | O | TYR | 85 | 33.943 | 16.977 | 58.495 | 1.00 | 37.44 | AAAA | O |
| ATOM | 848 | H | ALA | 86 | 33.027 | 15.691 | 59.979 | 1.00 | 30.21 | AAAA | N |
| ATOM | 850 | CA | ALA | 86 | 34.257 | 15.325 | 60.670 | 1.00 | 34.10 | AAAA | C |
| ATOM | 851 | CB | ALA | 86 | 33.999 | 15.370 | 62.157 | 1.00 | 25.48 | AAAA | C |
| ATOM | 852 | C | ALA | 86 | 34.729 | 13.962 | 60.216 | 1.00 | 32.67 | AAAA | C |
| ATOM | 853 | O | ALA | 86 | 35.795 | 13.481 | 60.577 | 1.00 | 35.10 | AAAA | O |
| ATOM | 854 | H | LEU | 87 | 33.832 | 13.173 | 59.597 | 1.00 | 28.56 | AAAA | N |
| ATOM | 856 | CA | LEU | 87 | 34.188 | 11.805 | 59.323 | 1.00 | 29.26 | AAAA | C |
| ATOM | 857 | CB | LEU | 87 | 33.798 | 10.860 | 60.471 | 1.00 | 13.64 | AAAA | C |
| ATOM | 858 | CG | LEU | 87 | 33.801 | 9.363 | 60.188 | 1.00 | 25.77 | AAAA | C |
| ATOM | 859 | CD1 | LEU | 87 | 35.140 | 8.915 | 59.571 | 1.00 | 27.21 | AAAA | C |
| ATOM | 860 | CD2 | LEU | 87 | 33.637 | 8.432 | 61.393 | 1.00 | 23.52 | AAAA | C |
| ATOM | 861 | C | LEU | 87 | 33.530 | 11.429 | 58.021 | 1.00 | 35.60 | AAAA | C |
| ATOM | 862 | O | LEU | 87 | 32.320 | 11.421 | 58.001 | 1.00 | 38.97 | AAAA | O |
| ATOM | 863 | H | VAL | 88 | 34.174 | 11.300 | 56.975 | 1.00 | 37.86 | AAAA | N |
| ATOM | 865 | CA | VAL | 88 | 33.438 | 11.032 | 55.628 | 1.00 | 33.32 | AAAA | C |
| ATOM | 866 | CB | VAL | 88 | 33.666 | 10.095 | 54.553 | 1.00 | 22.38 | AAAA | C |
| ATOM | 867 | CG1 | VAL | 88 | 32.974 | 11.675 | 53.261 | 1.00 | 19.24 | AAAA | C |
| ATOM | 868 | CG2 | VAL | 88 | 33.165 | 13.402 | 55.042 | 1.00 | 13.27 | AAAA | C |
| ATOM | 869 | C | VAL | 88 | 33.899 | 9.684 | 55.114 | 1.00 | 31.79 | AAAA | C |
| ATOM | 870 | O | VAL | 88 | 35.069 | 9.407 | 55.117 | 1.00 | 33.57 | AAAA | O |
| ATOM | 871 | H | ILE | 89 | 33.078 | 9.728 | 54.802 | 1.00 | 31.08 | AAAA | N |
| ATOM | 873 | CA | ILE | 89 | 33.361 | 7.433 | 54.280 | 1.00 | 30.45 | AAAA | C |
| ATOM | 874 | CB | ILE | 89 | 32.941 | 6.384 | 55.296 | 1.00 | 30.17 | AAAA | C |
| ATOM | 875 | CG2 | ILE | 89 | 32.898 | 4.954 | 54.921 | 1.00 | 37.24 | AAAA | C |
| ATOM | 876 | CG1 | ILE | 89 | 33.893 | 6.420 | 56.500 | 1.00 | 24.92 | AAAA | C |
| ATOM | 877 | CD1 | ILE | 89 | 33.424 | 5.613 | 57.675 | 1.00 | 23.96 | AAAA | C |
| ATOM | 878 | C | ILE | 89 | 32.509 | 7.206 | 53.027 | 1.00 | 40.64 | AAAA | C |
| ATOM | 879 | O | ILE | 89 | 31.330 | 6.891 | 53.205 | 1.00 | 38.69 | AAAA | O |
| ATOM | 880 | H | PHE | 90 | 33.082 | 7.464 | 51.845 | 1.00 | 41.45 | AAAA | N |
| ATOM | 882 | CA | PHE | 90 | 32.346 | 7.371 | 50.591 | 1.00 | 37.67 | AAAA | C |
| ATOM | 883 | CB | PHE | 90 | 32.347 | 8.776 | 50.110 | 1.00 | 32.17 | AAAA | C |
| ATOM | 884 | CG | PHE | 90 | 31.581 | 9.081 | 48.865 | 1.00 | 39.77 | AAAA | C |
| ATOM | 885 | CD1 | PHE | 90 | 30.387 | 9.772 | 49.025 | 1.00 | 32.02 | AAAA | C |
| ATOM | 886 | CD2 | PHE | 90 | 32.052 | 9.721 | 47.620 | 1.00 | 29.28 | AAAA | C |
| ATOM | 887 | CE1 | PHE | 90 | 29.611 | 10.111 | 47.938 | 1.00 | 33.30 | AAAA | C |
| ATOM | 888 | CE2 | PHE | 90 | 31.290 | 9.086 | 46.534 | 1.00 | 43.09 | AAAA | C |
| ATOM | 889 | CS | PHE | 90 | 30.083 | 9.764 | 46.687 | 1.00 | 50.24 | AAAA | C |
| ATOM | 890 | C | PHE | 90 | 32.856 | 6.384 | 49.557 | 1.00 | 40.72 | AAAA | C |
| ATOM | 891 | O | PHE | 90 | 34.027 | 6.296 | 49.203 | 1.00 | 46.15 | AAAA | O |
| ATOM | 892 | H | GLU | 91 | 32.024 | 5.519 | 49.001 | 1.00 | 39.16 | AAAA | N |
| ATOM | 894 | CA | GLU | 91 | 32.248 | 4.601 | 47.954 | 1.00 | 42.45 | AAAA | C |
| ATOM | 895 | CB | GLU | 91 | 32.479 | 5.231 | 46.583 | 1.00 | 38.08 | AAAA | C |
| ATOM | 896 | CG | GLU | 91 | 31.136 | 5.865 | 46.250 | 1.00 | 58.86 | AAAA | C |
| ATOM | 897 | CD | GLU | 91 | 30.855 | 5.776 | 44.757 | 1.00 | 63.55 | AAAA | C |
| ATOM | 898 | OE1 | GLU | 91 | 31.473 | 6.651 | 44.082 | 1.00 | 64.10 | AAAA | O |
| ATOM | 899 | OE2 | GLU | 91 | 30.058 | 4.813 | 44.573 | 1.00 | 63.64 | AAAA | O |
| ATOM | 900 | C | GLU | 91 | 33.422 | 3.734 | 48.313 | 1.00 | 42.06 | AAAA | C |
| ATOM | 901 | O | GLU | 91 | 34.298 | 3.411 | 47.587 | 1.00 | 44.71 | AAAA | O |
| ATOM | 902 | H | MET | 92 | 33.352 | 3.209 | 49.482 | 1.00 | 46.52 | AAAA | N |
| ATOM | 904 | CA | MET | 92 | 34.409 | 2.401 | 50.088 | 1.00 | 42.26 | AAAA | C |
| ATOM | 905 | CB | MET | 92 | 34.299 | 2.659 | 51.594 | 1.00 | 38.37 | AAAA | C |
| ATOM | 906 | CG | MET | 92 | 35.412 | 2.156 | 52.420 | 1.00 | 59.29 | AAAA | C |
| ATOM | 907 | SD | MET | 92 | 36.802 | 3.306 | 52.401 | 1.00 | 57.67 | AAAA | S |
| ATOM | 908 | CE | MET | 92 | 36.340 | 4.405 | 51.108 | 1.00 | 38.36 | AAAA | C |
| ATOM | 909 | C | MET | 92 | 34.012 | 1.005 | 49.745 | 1.00 | 43.37 | AAAA | C |
| ATOM | 910 | O | MET | 92 | 33.335 | 0.298 | 50.523 | 1.00 | 45.58 | AAAA | O |
| ATOM | 911 | H | THR | 93 | 34.449 | 0.518 | 48.602 | 1.00 | 47.09 | AAAA | N |
| ATOM | 913 | CA | THR | 93 | 34.175 | -0.900 | 48.273 | 1.00 | 47.32 | AAAA | C |
| ATOM | 914 | CB | THR | 93 | 34.666 | -1.281 | 46.868 | 1.00 | 55.28 | AAAA | C |
| ATOM | 915 | CG1 | THR | 93 | 34.013 | -0.488 | 45.892 | 1.00 | 57.81 | AAAA | O |
| ATOM | 917 | CG2 | THR | 93 | 34.332 | -2.715 | 46.516 | 1.00 | 44.71 | AAAA | C |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|---|
| ATOH | 912 | C | THR | 93 | 34.885 | -1.874 | 49.186 | 1.00 | 51.83 | AAAA | C |
| ATOH | 912 | O | THR | 93 | 36.115 | -1.777 | 49.361 | 1.00 | 57.91 | AAAA | O |
| ATOH | 920 | H | ASH | 94 | 34.237 | -2.983 | 49.493 | 1.00 | 49.85 | AAAA | H |
| ATOH | 922 | CA | ASH | 94 | 34.747 | -4.069 | 50.285 | 1.00 | 45.64 | AAAA | C |
| ATOH | 923 | CB | ASH | 94 | 36.241 | -4.315 | 50.001 | 1.00 | 59.01 | AAAA | C |
| ATOH | 924 | CG | ASH | 94 | 36.494 | -4.849 | 48.599 | 1.00 | 75.44 | AAAA | C |
| ATOH | 925 | OD1 | ASH | 94 | 36.847 | -4.081 | 47.688 | 1.00 | 77.49 | AAAA | O |
| ATOH | 926 | HD2 | ASH | 94 | 36.308 | -6.153 | 48.408 | 1.00 | 79.63 | AAAA | H |
| ATOH | 929 | C | ASH | 94 | 34.522 | -3.838 | 51.763 | 1.00 | 42.58 | AAAA | C |
| ATOH | 930 | O | ASH | 94 | 34.752 | -4.814 | 52.501 | 1.00 | 46.36 | AAAA | O |
| ATOH | 931 | H | LEU | 95 | 34.308 | -2.609 | 52.182 | 1.00 | 37.28 | AAAA | H |
| ATOH | 933 | CA | LEU | 95 | 34.324 | -2.277 | 53.621 | 1.00 | 39.96 | AAAA | C |
| ATOH | 934 | CB | LEU | 95 | 34.185 | -0.786 | 53.851 | 1.00 | 34.05 | AAAA | C |
| ATOH | 935 | CG | LEU | 95 | 34.323 | -0.296 | 55.269 | 1.00 | 35.81 | AAAA | C |
| ATOH | 936 | CD1 | LEU | 95 | 35.785 | -0.537 | 55.598 | 1.00 | 35.48 | AAAA | C |
| ATOH | 937 | CD2 | LEU | 95 | 33.847 | 1.177 | 55.344 | 1.00 | 25.46 | AAAA | C |
| ATOH | 938 | C | LEU | 95 | 33.163 | -2.986 | 54.275 | 1.00 | 43.75 | AAAA | C |
| ATOH | 939 | O | LEU | 95 | 32.048 | -2.936 | 53.772 | 1.00 | 44.04 | AAAA | O |
| ATOH | 940 | H | LYS | 96 | 33.451 | -3.863 | 55.213 | 1.00 | 46.50 | AAAA | H |
| ATOH | 942 | CA | LYS | 96 | 32.364 | -4.649 | 55.779 | 1.00 | 42.76 | AAAA | C |
| ATOH | 943 | CB | LYS | 96 | 32.801 | -6.075 | 55.995 | 1.00 | 41.41 | AAAA | C |
| ATOH | 944 | CG | LYS | 96 | 32.760 | -6.976 | 54.788 | 1.00 | 49.78 | AAAA | C |
| ATOH | 945 | CD | LYS | 96 | 32.984 | -8.446 | 55.127 | 1.00 | 58.09 | AAAA | C |
| ATOH | 946 | CE | LYS | 96 | 33.772 | -9.160 | 54.027 | 1.00 | 73.43 | AAAA | C |
| ATOH | 947 | NE | LYS | 96 | 34.098 | -10.556 | 54.489 | 1.00 | 79.13 | AAAA | N |
| ATOH | 951 | C | LYS | 96 | 31.970 | -4.055 | 57.122 | 1.00 | 45.29 | AAAA | C |
| ATOH | 952 | O | LYS | 96 | 30.978 | -4.502 | 57.691 | 1.00 | 46.23 | AAAA | O |
| ATOH | 953 | H | ASP | 97 | 32.685 | -3.071 | 57.645 | 1.00 | 45.15 | AAAA | H |
| ATOH | 955 | CA | ASP | 97 | 32.299 | -2.384 | 58.861 | 1.00 | 42.15 | AAAA | C |
| ATOH | 956 | CB | ASP | 97 | 32.294 | -3.292 | 60.059 | 1.00 | 45.39 | AAAA | C |
| ATOH | 957 | CG | ASP | 97 | 33.662 | -3.562 | 60.624 | 1.00 | 56.95 | AAAA | C |
| ATOH | 958 | OD1 | ASP | 97 | 34.579 | -2.825 | 61.012 | 1.00 | 59.88 | AAAA | O |
| ATOH | 959 | OD2 | ASP | 97 | 33.931 | -4.782 | 60.714 | 1.00 | 56.01 | AAAA | O |
| ATOH | 960 | C | ASP | 97 | 33.209 | -1.224 | 59.201 | 1.00 | 41.25 | AAAA | C |
| ATOH | 961 | O | ASP | 97 | 34.160 | -1.074 | 58.437 | 1.00 | 47.03 | AAAA | O |
| ATOH | 962 | H | ILE | 98 | 32.922 | -0.366 | 60.129 | 1.00 | 40.41 | AAAA | H |
| ATOH | 964 | CA | ILE | 98 | 33.675 | 0.820 | 60.340 | 1.00 | 37.83 | AAAA | C |
| ATOH | 965 | CB | ILE | 98 | 32.983 | 2.006 | 61.006 | 1.00 | 38.99 | AAAA | C |
| ATOH | 966 | CD1 | ILE | 98 | 34.007 | 3.133 | 61.207 | 1.00 | 38.95 | AAAA | C |
| ATOH | 967 | CD2 | ILE | 98 | 31.835 | 2.489 | 60.092 | 1.00 | 34.84 | AAAA | C |
| ATOH | 968 | CE1 | ILE | 98 | 31.629 | 3.959 | 59.948 | 1.00 | 39.29 | AAAA | C |
| ATOH | 969 | C | ILE | 98 | 34.854 | 0.322 | 61.114 | 1.00 | 35.11 | AAAA | C |
| ATOH | 970 | O | ILE | 98 | 35.970 | 0.669 | 60.841 | 1.00 | 43.05 | AAAA | O |
| ATOH | 971 | H | GLY | 99 | 34.619 | -0.393 | 62.192 | 1.00 | 34.22 | AAAA | H |
| ATOH | 973 | CA | GLY | 99 | 35.477 | -0.972 | 63.121 | 1.00 | 33.74 | AAAA | C |
| ATOH | 974 | C | GLY | 99 | 36.279 | -0.084 | 64.024 | 1.00 | 35.90 | AAAA | C |
| ATOH | 975 | O | GLY | 99 | 37.023 | -0.572 | 64.899 | 1.00 | 38.21 | AAAA | O |
| ATOH | 976 | H | LEU | 100 | 36.120 | 1.321 | 63.913 | 1.00 | 33.35 | AAAA | H |
| ATOH | 978 | CA | LEU | 100 | 36.763 | 2.215 | 64.771 | 1.00 | 31.65 | AAAA | C |
| ATOH | 979 | CB | LEU | 100 | 36.496 | 3.636 | 64.294 | 1.00 | 29.87 | AAAA | C |
| ATOH | 980 | CG | LEU | 100 | 36.943 | 3.980 | 62.835 | 1.00 | 32.13 | AAAA | C |
| ATOH | 991 | CD1 | LEU | 100 | 36.710 | 5.479 | 62.610 | 1.00 | 21.38 | AAAA | C |
| ATOH | 992 | CD2 | LEU | 100 | 38.412 | 3.599 | 62.644 | 1.00 | 37.68 | AAAA | C |
| ATOH | 993 | C | LEU | 100 | 36.312 | 1.976 | 66.194 | 1.00 | 31.94 | AAAA | C |
| ATOH | 994 | O | LEU | 100 | 35.950 | 2.863 | 66.979 | 1.00 | 31.95 | AAAA | O |
| ATOH | 995 | H | TYR | 101 | 36.704 | 0.851 | 66.779 | 1.00 | 31.87 | AAAA | H |
| ATOH | 997 | CA | TYR | 101 | 36.329 | 0.395 | 68.071 | 1.00 | 33.33 | AAAA | C |
| ATOH | 998 | CB | TYR | 101 | 36.491 | -1.104 | 68.264 | 1.00 | 41.03 | AAAA | C |
| ATOH | 999 | CG | TYR | 101 | 37.919 | -1.559 | 68.369 | 1.00 | 46.66 | AAAA | C |
| ATOH | 990 | CD1 | TYR | 101 | 38.571 | -1.380 | 69.587 | 1.00 | 51.20 | AAAA | C |
| ATOH | 991 | CE1 | TYR | 101 | 39.901 | -1.743 | 69.749 | 1.00 | 49.44 | AAAA | C |
| ATOH | 992 | CD2 | TYR | 101 | 38.615 | -2.112 | 67.322 | 1.00 | 45.15 | AAAA | C |
| ATOH | 993 | CE2 | TYR | 101 | 39.927 | -2.505 | 67.479 | 1.00 | 47.08 | AAAA | C |
| ATOH | 994 | CC | TYR | 101 | 40.548 | -2.321 | 68.688 | 1.00 | 49.43 | AAAA | C |
| ATOH | 995 | OH | TYR | 101 | 41.834 | -2.662 | 68.997 | 1.00 | 55.82 | AAAA | O |
| ATOH | 997 | C | TYR | 101 | 36.989 | 1.059 | 69.214 | 1.00 | 33.46 | AAAA | C |
| ATOH | 998 | O | TYR | 101 | 36.630 | 0.813 | 70.375 | 1.00 | 43.00 | AAAA | O |
| ATOH | 999 | H | ASH | 102 | 37.752 | 2.091 | 69.068 | 1.00 | 38.12 | AAAA | N |
| ATOH | 1001 | CA | ASH | 102 | 38.093 | 2.979 | 70.223 | 1.00 | 30.78 | AAAA | C |
| ATOH | 1002 | CB | ASH | 102 | 39.603 | 2.911 | 70.363 | 1.00 | 48.63 | AAAA | C |
| ATOH | 1003 | CG | ASH | 102 | 40.112 | 1.904 | 71.268 | 1.00 | 54.01 | AAAA | C |
| ATOH | 1004 | OD1 | ASH | 102 | 39.738 | 1.864 | 72.454 | 1.00 | 47.22 | AAAA | O |
| ATOH | 1005 | HD2 | ASH | 102 | 40.864 | 0.845 | 70.767 | 1.00 | 43.08 | AAAA | H |
| ATOH | 1008 | C | ASH | 102 | 37.673 | 4.385 | 69.947 | 1.00 | 33.82 | AAAA | C |
| ATOH | 1009 | O | ASH | 102 | 38.047 | 5.364 | 70.592 | 1.00 | 39.84 | AAAA | O |
| ATOH | 1010 | H | LEU | 103 | 36.845 | 4.640 | 68.882 | 1.00 | 35.28 | AAAA | H |
| ATOH | 1012 | CA | LEU | 103 | 36.473 | 6.040 | 68.621 | 1.00 | 36.57 | AAAA | C |
| ATOH | 1013 | CB | LEU | 103 | 35.948 | 6.140 | 67.213 | 1.00 | 34.77 | AAAA | C |
| ATOH | 1014 | CG | LEU | 103 | 35.525 | 7.492 | 66.612 | 1.00 | 30.32 | AAAA | C |
| ATOH | 1015 | CD1 | LEU | 103 | 36.606 | 8.513 | 66.646 | 1.00 | 23.20 | AAAA | C |
| ATOH | 1016 | CD2 | LEU | 103 | 35.198 | 7.169 | 65.146 | 1.00 | 37.10 | AAAA | C |
| ATOH | 1017 | C | LEU | 103 | 35.484 | 6.508 | 69.691 | 1.00 | 37.31 | AAAA | C |
| ATOH | 1019 | O | LEU | 103 | 34.449 | 5.874 | 69.837 | 1.00 | 34.24 | AAAA | O |
| ATOH | 1019 | H | ARG | 104 | 35.810 | 7.456 | 70.563 | 1.00 | 33.31 | AAAA | H |
| ATOH | 1021 | CA | ARG | 104 | 34.920 | 7.841 | 71.605 | 1.00 | 29.86 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 1022 | CB | ARG | 104 | 35.589 | 7.657 | 73.019 | 1.00 | 38.17 | AAAA | C |
| ATOM | 1023 | CG | ARG | 104 | 36.356 | 6.375 | 73.165 | 1.00 | 48.37 | AAAA | C |
| ATOM | 1024 | CD | ARG | 104 | 35.425 | 5.183 | 73.248 | 1.00 | 50.71 | AAAA | C |
| ATOM | 1025 | HE | ARG | 104 | 34.582 | 5.320 | 74.413 | 1.00 | 52.38 | AAAA | N |
| ATOM | 1027 | CG | ARG | 104 | 34.900 | 4.847 | 75.621 | 1.00 | 72.73 | AAAA | C |
| ATOM | 1028 | HH1 | ARG | 104 | 36.047 | 4.214 | 75.800 | 1.00 | 81.87 | AAAA | N |
| ATOM | 1031 | HH2 | ARG | 104 | 33.990 | 5.070 | 76.577 | 1.00 | 78.27 | AAAA | N |
| ATOM | 1034 | C | ARG | 104 | 34.466 | 9.273 | 71.540 | 1.00 | 32.58 | AAAA | C |
| ATOM | 1035 | O | ARG | 104 | 33.553 | 9.743 | 72.223 | 1.00 | 39.89 | AAAA | O |
| ATOM | 1036 | H | ASH | 105 | 34.992 | 10.065 | 70.637 | 1.00 | 33.47 | AAAA | H |
| ATOM | 1038 | CA | ASH | 105 | 34.549 | 11.450 | 70.590 | 1.00 | 30.97 | AAAA | C |
| ATOM | 1044 | C | ASH | 105 | 34.907 | 12.149 | 69.310 | 1.00 | 31.00 | AAAA | C |
| ATOM | 1045 | O | ASH | 105 | 36.086 | 12.067 | 69.050 | 1.00 | 37.79 | AAAA | O |
| ATOM | 1039 | CB | ASH | 105 | 35.203 | 12.199 | 71.721 | 1.00 | 12.28 | AAAA | C |
| ATOM | 1040 | CG | ASH | 105 | 34.786 | 13.568 | 71.756 | 1.00 | 24.93 | AAAA | C |
| ATOM | 1041 | OD1 | ASH | 105 | 35.125 | 14.549 | 71.127 | 1.00 | 38.14 | AAAA | O |
| ATOM | 1042 | HD2 | ASH | 105 | 33.828 | 13.985 | 72.649 | 1.00 | 35.96 | AAAA | N |
| ATOM | 1046 | N | ILE | 106 | 33.969 | 12.669 | 68.576 | 1.00 | 31.90 | AAAA | N |
| ATOM | 1048 | CA | ILE | 106 | 34.129 | 13.551 | 67.469 | 1.00 | 23.39 | AAAA | C |
| ATOM | 1049 | CB | ILE | 106 | 33.239 | 13.185 | 66.307 | 1.00 | 16.54 | AAAA | C |
| ATOM | 1050 | CG2 | ILE | 106 | 33.132 | 14.408 | 65.374 | 1.00 | 20.38 | AAAA | C |
| ATOM | 1051 | CG1 | ILE | 106 | 33.928 | 12.034 | 65.558 | 1.00 | 18.30 | AAAA | C |
| ATOM | 1052 | CD1 | ILE | 106 | 33.055 | 11.293 | 64.643 | 1.00 | 25.48 | AAAA | C |
| ATOM | 1053 | C | ILE | 106 | 33.803 | 14.909 | 68.009 | 1.00 | 27.40 | AAAA | C |
| ATOM | 1054 | O | ILE | 106 | 32.628 | 15.106 | 68.243 | 1.00 | 32.86 | AAAA | O |
| ATOM | 1055 | H | THR | 107 | 34.719 | 15.789 | 68.350 | 1.00 | 30.43 | AAAA | H |
| ATOM | 1057 | CA | THR | 107 | 34.532 | 16.983 | 69.145 | 1.00 | 28.27 | AAAA | C |
| ATOM | 1058 | CB | THR | 107 | 35.902 | 17.607 | 69.579 | 1.00 | 35.78 | AAAA | C |
| ATOM | 1059 | OG1 | THR | 107 | 36.819 | 16.503 | 69.738 | 1.00 | 40.26 | AAAA | O |
| ATOM | 1061 | CG2 | THR | 107 | 35.954 | 18.411 | 70.855 | 1.00 | 28.13 | AAAA | C |
| ATOM | 1062 | C | THR | 107 | 33.728 | 17.950 | 68.332 | 1.00 | 27.95 | AAAA | C |
| ATOM | 1063 | O | THR | 107 | 33.392 | 19.060 | 68.831 | 1.00 | 32.99 | AAAA | O |
| ATOM | 1064 | H | ARG | 108 | 33.669 | 17.777 | 67.019 | 1.00 | 30.28 | AAAA | N |
| ATOM | 1066 | CA | ARG | 108 | 33.046 | 18.809 | 66.180 | 1.00 | 31.25 | AAAA | C |
| ATOM | 1067 | CB | ARG | 108 | 33.965 | 20.011 | 65.951 | 1.00 | 25.13 | AAAA | C |
| ATOM | 1068 | CG | ARG | 108 | 33.105 | 21.174 | 65.543 | 1.00 | 30.68 | AAAA | C |
| ATOM | 1069 | CD | ARG | 108 | 33.917 | 22.444 | 65.529 | 1.00 | 17.12 | AAAA | C |
| ATOM | 1070 | HE | ARG | 108 | 33.511 | 23.376 | 64.451 | 1.00 | 33.40 | AAAA | N |
| ATOM | 1071 | CG | ARG | 108 | 34.045 | 23.608 | 63.266 | 1.00 | 46.41 | AAAA | C |
| ATOM | 1073 | HH1 | ARG | 108 | 35.162 | 22.929 | 62.868 | 1.00 | 40.30 | AAAA | H |
| ATOM | 1076 | HH2 | ARG | 108 | 33.454 | 24.543 | 62.494 | 1.00 | 39.82 | AAAA | H |
| ATOM | 1079 | C | ARG | 108 | 32.701 | 19.328 | 64.784 | 1.00 | 31.50 | AAAA | C |
| ATOM | 1080 | O | ARG | 108 | 33.379 | 17.391 | 64.430 | 1.00 | 32.67 | AAAA | O |
| ATOM | 1081 | H | GLY | 109 | 31.567 | 19.909 | 64.284 | 1.00 | 32.60 | AAAA | H |
| ATOM | 1083 | CA | GLY | 109 | 31.082 | 19.395 | 62.983 | 1.00 | 28.87 | AAAA | C |
| ATOM | 1084 | C | GLY | 109 | 30.470 | 17.008 | 63.001 | 1.00 | 32.32 | AAAA | C |
| ATOM | 1085 | O | GLY | 109 | 30.471 | 16.306 | 64.006 | 1.00 | 38.03 | AAAA | O |
| ATOM | 1086 | H | ALA | 110 | 29.920 | 16.560 | 61.894 | 1.00 | 34.11 | AAAA | N |
| ATOM | 1089 | CA | ALA | 110 | 29.086 | 15.371 | 61.833 | 1.00 | 36.77 | AAAA | C |
| ATOM | 1089 | CB | ALA | 110 | 27.702 | 15.701 | 61.223 | 1.00 | 15.32 | AAAA | C |
| ATOM | 1090 | C | ALA | 110 | 29.745 | 14.335 | 60.957 | 1.00 | 32.12 | AAAA | C |
| ATOM | 1091 | O | ALA | 110 | 30.921 | 14.332 | 60.687 | 1.00 | 34.11 | AAAA | O |
| ATOM | 1092 | H | ILE | 111 | 29.030 | 13.337 | 60.557 | 1.00 | 26.55 | AAAA | H |
| ATOM | 1094 | CA | ILE | 111 | 29.569 | 12.273 | 59.771 | 1.00 | 32.90 | AAAA | C |
| ATOM | 1095 | CB | ILE | 111 | 29.669 | 10.967 | 60.591 | 1.00 | 38.07 | AAAA | C |
| ATOM | 1096 | CG2 | ILE | 111 | 30.091 | 11.140 | 62.036 | 1.00 | 34.05 | AAAA | C |
| ATOM | 1097 | CG1 | ILE | 111 | 28.345 | 10.237 | 60.684 | 1.00 | 26.54 | AAAA | C |
| ATOM | 1098 | CD1 | ILE | 111 | 28.437 | 8.872 | 61.407 | 1.00 | 27.11 | AAAA | C |
| ATOM | 1099 | C | ILE | 111 | 28.738 | 11.928 | 58.521 | 1.00 | 33.98 | AAAA | C |
| ATOM | 1100 | O | ILE | 111 | 27.533 | 12.179 | 58.532 | 1.00 | 32.15 | AAAA | O |
| ATOM | 1101 | H | ARG | 112 | 29.432 | 11.423 | 57.501 | 1.00 | 30.54 | AAAA | H |
| ATOM | 1103 | CA | ARG | 112 | 28.773 | 11.107 | 56.247 | 1.00 | 27.48 | AAAA | C |
| ATOM | 1104 | CB | ARG | 112 | 29.186 | 12.085 | 55.169 | 1.00 | 26.35 | AAAA | C |
| ATOM | 1105 | CG | ARG | 112 | 28.548 | 11.653 | 53.816 | 1.00 | 25.93 | AAAA | C |
| ATOM | 1106 | CD | ARG | 112 | 28.659 | 12.912 | 52.992 | 1.00 | 32.92 | AAAA | C |
| ATOM | 1107 | HE | ARG | 112 | 27.950 | 12.726 | 51.770 | 1.00 | 50.34 | AAAA | H |
| ATOM | 1109 | CG | ARG | 112 | 27.778 | 13.503 | 50.720 | 1.00 | 47.61 | AAAA | C |
| ATOM | 1110 | HH1 | ARG | 112 | 28.334 | 14.695 | 50.696 | 1.00 | 44.92 | AAAA | H |
| ATOM | 1113 | HH2 | ARG | 112 | 27.012 | 12.925 | 49.789 | 1.00 | 46.00 | AAAA | H |
| ATOM | 1116 | C | ARG | 112 | 29.200 | 9.738 | 55.791 | 1.00 | 29.74 | AAAA | C |
| ATOM | 1117 | O | ARG | 112 | 30.343 | 9.611 | 55.406 | 1.00 | 36.52 | AAAA | O |
| ATOM | 1118 | N | ILE | 113 | 28.326 | 9.754 | 55.886 | 1.00 | 33.99 | AAAA | N |
| ATOM | 1120 | CA | ILE | 113 | 28.612 | 7.376 | 55.555 | 1.00 | 36.26 | AAAA | C |
| ATOM | 1121 | CB | ILE | 113 | 28.457 | 6.461 | 56.760 | 1.00 | 33.27 | AAAA | C |
| ATOM | 1122 | CG2 | ILE | 113 | 28.850 | 5.021 | 56.449 | 1.00 | 15.95 | AAAA | C |
| ATOM | 1123 | CG1 | ILE | 113 | 29.374 | 7.012 | 57.874 | 1.00 | 31.92 | AAAA | C |
| ATOM | 1124 | CD1 | ILE | 113 | 29.324 | 6.250 | 59.176 | 1.00 | 42.34 | AAAA | C |
| ATOM | 1125 | C | ILE | 113 | 27.729 | 6.959 | 54.398 | 1.00 | 39.26 | AAAA | C |
| ATOM | 1126 | O | ILE | 113 | 26.637 | 6.482 | 54.664 | 1.00 | 50.72 | AAAA | O |
| ATOM | 1127 | N | GLU | 114 | 28.175 | 7.199 | 53.190 | 1.00 | 35.86 | AAAA | H |
| ATOM | 1129 | CA | GLU | 114 | 27.491 | 7.103 | 51.935 | 1.00 | 38.76 | AAAA | C |
| ATOM | 1130 | CB | GLU | 114 | 27.471 | 8.443 | 51.216 | 1.00 | 25.58 | AAAA | C |
| ATOM | 1131 | CG | GLU | 114 | 26.567 | 8.402 | 49.969 | 1.00 | 27.97 | AAAA | C |
| ATOM | 1132 | CD | GLU | 114 | 26.349 | 9.840 | 49.578 | 1.00 | 36.85 | AAAA | C |
| ATOM | 1133 | OE1 | GLU | 114 | 26.763 | 10.662 | 50.414 | 1.00 | 45.57 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 1134 | OE1 | GLU | 114 | 25.787 | 10.106 | 48.488 | 1.00 | 35.53 | AAAA | O |
| ATOH | 1135 | C | GLU | 114 | 29.039 | 6.072 | 50.944 | 1.00 | 44.17 | AAAA | C |
| ATOH | 1136 | O | GLU | 114 | 29.120 | 5.538 | 51.090 | 1.00 | 49.97 | AAAA | O |
| ATOH | 1137 | H | LYS | 115 | 27.191 | 5.556 | 50.096 | 1.00 | 40.55 | AAAA | N |
| ATOH | 1139 | CA | LYS | 115 | 27.219 | 4.440 | 49.242 | 1.00 | 41.16 | AAAA | C |
| ATOH | 1140 | CB | LYS | 115 | 27.275 | 4.764 | 47.718 | 1.00 | 23.62 | AAAA | C |
| ATOH | 1141 | CG | LYS | 115 | 27.019 | 6.194 | 47.411 | 1.00 | 18.39 | AAAA | C |
| ATOH | 1142 | CD | LYS | 115 | 26.537 | 6.355 | 45.982 | 1.00 | 24.74 | AAAA | C |
| ATOH | 1143 | CE | LYS | 115 | 26.751 | 7.804 | 45.622 | 1.00 | 41.86 | AAAA | C |
| ATOH | 1144 | HE | LYS | 115 | 27.165 | 8.045 | 44.196 | 1.00 | 60.91 | AAAA | N |
| ATOH | 1148 | C | LYS | 115 | 28.287 | 3.421 | 49.611 | 1.00 | 42.39 | AAAA | C |
| ATOH | 1149 | O | LYS | 115 | 29.102 | 3.103 | 48.749 | 1.00 | 46.68 | AAAA | O |
| ATOH | 1150 | H | ASN | 116 | 28.137 | 2.677 | 50.665 | 1.00 | 40.99 | AAAA | N |
| ATOH | 1152 | CA | ASN | 116 | 29.022 | 1.570 | 50.976 | 1.00 | 37.33 | AAAA | C |
| ATOH | 1153 | CB | ASN | 116 | 29.534 | 1.868 | 52.381 | 1.00 | 46.12 | AAAA | C |
| ATOH | 1154 | CG | ASN | 116 | 30.372 | 3.153 | 52.345 | 1.00 | 48.92 | AAAA | C |
| ATOH | 1155 | OD1 | ASN | 116 | 31.337 | 3.016 | 51.583 | 1.00 | 38.59 | AAAA | O |
| ATOH | 1156 | HD2 | ASN | 116 | 29.927 | 4.174 | 53.056 | 1.00 | 37.35 | AAAA | N |
| ATOH | 1159 | C | ASN | 116 | 28.275 | 0.277 | 50.974 | 1.00 | 42.52 | AAAA | C |
| ATOH | 1160 | O | ASN | 116 | 28.067 | -0.361 | 52.033 | 1.00 | 48.24 | AAAA | O |
| ATOH | 1161 | H | ALA | 117 | 27.989 | -0.188 | 49.772 | 1.00 | 40.94 | AAAA | N |
| ATOH | 1163 | CA | ALA | 117 | 27.195 | -1.376 | 49.542 | 1.00 | 43.35 | AAAA | C |
| ATOH | 1164 | CB | ALA | 117 | 27.494 | -1.884 | 48.156 | 1.00 | 47.63 | AAAA | C |
| ATOH | 1165 | C | ALA | 117 | 27.294 | -2.504 | 50.529 | 1.00 | 46.55 | AAAA | C |
| ATOH | 1166 | O | ALA | 117 | 26.211 | -2.998 | 50.890 | 1.00 | 51.24 | AAAA | O |
| ATOH | 1167 | H | ASP | 118 | 28.484 | -2.823 | 51.005 | 1.00 | 47.43 | AAAA | N |
| ATOH | 1169 | CA | ASP | 118 | 28.559 | -3.980 | 51.920 | 1.00 | 45.74 | AAAA | C |
| ATOH | 1170 | CB | ASP | 118 | 29.659 | -4.945 | 51.477 | 1.00 | 55.39 | AAAA | C |
| ATOH | 1171 | CG | ASP | 118 | 29.684 | -5.119 | 49.958 | 1.00 | 59.40 | AAAA | C |
| ATOH | 1172 | OD1 | ASP | 118 | 28.870 | -5.976 | 49.608 | 1.00 | 64.40 | AAAA | O |
| ATOH | 1173 | OD2 | ASP | 118 | 30.448 | -4.447 | 49.207 | 1.00 | 66.73 | AAAA | O |
| ATOH | 1174 | C | ASP | 118 | 28.818 | -3.586 | 53.353 | 1.00 | 37.29 | AAAA | C |
| ATOH | 1175 | O | ASP | 118 | 29.127 | -4.536 | 54.026 | 1.00 | 42.89 | AAAA | O |
| ATOH | 1176 | H | LEU | 119 | 28.670 | -2.327 | 53.685 | 1.00 | 36.46 | AAAA | N |
| ATOH | 1178 | CA | LEU | 119 | 28.986 | -1.895 | 55.047 | 1.00 | 40.58 | AAAA | C |
| ATOH | 1179 | CB | LEU | 119 | 29.159 | -0.389 | 55.145 | 1.00 | 34.31 | AAAA | C |
| ATOH | 1180 | CG | LEU | 119 | 29.640 | 0.331 | 56.378 | 1.00 | 36.58 | AAAA | C |
| ATOH | 1181 | OD1 | LEU | 119 | 30.950 | -0.101 | 56.948 | 1.00 | 35.77 | AAAA | C |
| ATOH | 1182 | OD2 | LEU | 119 | 29.791 | 1.830 | 56.104 | 1.00 | 29.68 | AAAA | C |
| ATOH | 1183 | C | LEU | 119 | 27.937 | -2.376 | 56.007 | 1.00 | 43.67 | AAAA | C |
| ATOH | 1184 | O | LEU | 119 | 26.748 | -2.248 | 55.743 | 1.00 | 45.32 | AAAA | O |
| ATOH | 1185 | H | CYS | 120 | 28.361 | -2.967 | 57.110 | 1.00 | 43.53 | AAAA | N |
| ATOH | 1187 | CA | CYS | 120 | 27.378 | -3.407 | 59.089 | 1.00 | 38.93 | AAAA | C |
| ATOH | 1188 | C | CYS | 120 | 27.981 | -3.921 | 59.426 | 1.00 | 41.91 | AAAA | C |
| ATOH | 1189 | O | CYS | 120 | 28.660 | -1.960 | 59.446 | 1.00 | 43.66 | AAAA | O |
| ATOH | 1190 | CB | CYS | 120 | 27.285 | -4.907 | 59.100 | 1.00 | 37.59 | AAAA | C |
| ATOH | 1191 | SG | CYS | 120 | 26.568 | -5.622 | 56.639 | 1.00 | 58.32 | AAAA | S |
| ATOH | 1192 | H | TYR | 121 | 27.328 | -3.456 | 60.509 | 1.00 | 38.05 | AAAA | N |
| ATOH | 1194 | CA | TYR | 121 | 27.795 | -3.010 | 61.927 | 1.00 | 38.68 | AAAA | C |
| ATOH | 1195 | CB | TYR | 121 | 29.189 | -3.572 | 62.130 | 1.00 | 34.61 | AAAA | C |
| ATOH | 1196 | CG | TYR | 121 | 28.950 | -5.032 | 62.519 | 1.00 | 36.52 | AAAA | C |
| ATOH | 1197 | OD1 | TYR | 121 | 29.087 | -6.045 | 61.582 | 1.00 | 33.58 | AAAA | C |
| ATOH | 1198 | CE1 | TYR | 121 | 28.852 | -7.350 | 61.980 | 1.00 | 41.21 | AAAA | C |
| ATOH | 1199 | CD2 | TYR | 121 | 28.560 | -5.337 | 63.817 | 1.00 | 36.31 | AAAA | C |
| ATOH | 1200 | CE2 | TYR | 121 | 28.287 | -6.630 | 64.201 | 1.00 | 39.49 | AAAA | C |
| ATOH | 1201 | CE | TYR | 121 | 28.432 | -7.641 | 63.270 | 1.00 | 46.07 | AAAA | C |
| ATOH | 1202 | OH | TYR | 121 | 28.161 | -8.924 | 63.730 | 1.00 | 49.20 | AAAA | O |
| ATOH | 1204 | C | TYR | 121 | 27.674 | -1.523 | 61.789 | 1.00 | 38.83 | AAAA | C |
| ATOH | 1205 | O | TYR | 121 | 28.445 | -0.778 | 62.369 | 1.00 | 43.22 | AAAA | O |
| ATOH | 1206 | H | LEU | 122 | 26.587 | -1.045 | 61.180 | 1.00 | 39.58 | AAAA | N |
| ATOH | 1208 | CA | LEU | 122 | 26.361 | 0.405 | 61.090 | 1.00 | 44.82 | AAAA | C |
| ATOH | 1209 | CB | LEU | 122 | 25.990 | 0.715 | 59.634 | 1.00 | 46.48 | AAAA | C |
| ATOH | 1210 | CG | LEU | 122 | 26.497 | 2.014 | 59.108 | 1.00 | 44.44 | AAAA | C |
| ATOH | 1211 | CD1 | LEU | 122 | 25.778 | 2.448 | 57.859 | 1.00 | 32.19 | AAAA | C |
| ATOH | 1212 | CD2 | LEU | 122 | 26.136 | 3.057 | 60.170 | 1.00 | 47.76 | AAAA | C |
| ATOH | 1213 | C | LEU | 122 | 25.212 | 0.910 | 61.935 | 1.00 | 44.85 | AAAA | C |
| ATOH | 1214 | O | LEU | 122 | 25.269 | 1.759 | 62.839 | 1.00 | 47.66 | AAAA | O |
| ATOH | 1215 | H | SER | 123 | 24.104 | 0.137 | 61.843 | 1.00 | 40.12 | AAAA | N |
| ATOH | 1217 | CA | SER | 123 | 22.949 | 0.435 | 62.703 | 1.00 | 33.98 | AAAA | C |
| ATOH | 1218 | CB | SER | 123 | 21.754 | -0.330 | 62.239 | 1.00 | 19.26 | AAAA | C |
| ATOH | 1219 | OG | SER | 123 | 21.964 | -1.762 | 62.402 | 1.00 | 34.35 | AAAA | O |
| ATOH | 1221 | C | SER | 123 | 23.165 | 0.060 | 64.159 | 1.00 | 37.43 | AAAA | C |
| ATOH | 1222 | O | SER | 123 | 22.326 | 0.280 | 65.025 | 1.00 | 35.33 | AAAA | O |
| ATOH | 1223 | H | THR | 124 | 24.242 | -0.698 | 64.432 | 1.00 | 39.03 | AAAA | N |
| ATOH | 1225 | CA | THR | 124 | 24.554 | -1.165 | 65.753 | 1.00 | 37.78 | AAAA | C |
| ATOH | 1226 | CB | THR | 124 | 25.368 | -2.461 | 65.719 | 1.00 | 42.39 | AAAA | C |
| ATOH | 1227 | OG1 | THR | 124 | 26.502 | -2.020 | 64.924 | 1.00 | 47.70 | AAAA | O |
| ATOH | 1229 | CG2 | THR | 124 | 24.677 | -3.622 | 65.006 | 1.00 | 40.93 | AAAA | C |
| ATOH | 1230 | C | THR | 124 | 25.522 | -0.206 | 66.445 | 1.00 | 39.29 | AAAA | C |
| ATOH | 1231 | O | THR | 124 | 25.948 | -0.642 | 67.499 | 1.00 | 41.41 | AAAA | O |
| ATOH | 1232 | H | VAL | 125 | 25.737 | 1.001 | 65.985 | 1.00 | 37.80 | AAAA | N |
| ATOH | 1234 | CA | VAL | 125 | 26.594 | 1.964 | 66.661 | 1.00 | 41.06 | AAAA | C |
| ATOH | 1235 | CB | VAL | 125 | 27.683 | 2.542 | 65.714 | 1.00 | 39.50 | AAAA | C |
| ATOH | 1236 | CG1 | VAL | 125 | 28.570 | 3.599 | 66.352 | 1.00 | 28.36 | AAAA | C |
| ATOH | 1237 | CG2 | VAL | 125 | 28.693 | 1.565 | 65.110 | 1.00 | 33.07 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 1234 | C | VAL | 125 | 25.759 | 3.127 | 67.179 | 1.00 | 41.17 | AAAA | C |
| ATOH | 1235 | O | VAL | 125 | 24.941 | 3.750 | 66.531 | 1.00 | 41.22 | AAAA | O |
| ATOH | 1240 | H | ASP | 126 | 26.072 | 3.636 | 68.367 | 1.00 | 44.54 | AAAA | H |
| ATOH | 1242 | CA | ASP | 126 | 25.310 | 4.734 | 68.967 | 1.00 | 37.44 | AAAA | C |
| ATOH | 1243 | CB | ASP | 126 | 24.862 | 4.335 | 70.342 | 1.00 | 34.73 | AAAA | C |
| ATOH | 1244 | CG | ASP | 126 | 23.879 | 5.303 | 70.983 | 1.00 | 45.53 | AAAA | C |
| ATOH | 1245 | OD1 | ASP | 126 | 23.699 | 6.520 | 70.685 | 1.00 | 27.71 | AAAA | O |
| ATOH | 1246 | OD2 | ASP | 126 | 23.220 | 4.865 | 71.964 | 1.00 | 52.32 | AAAA | O |
| ATOH | 1247 | C | ASP | 126 | 26.146 | 5.985 | 68.872 | 1.00 | 40.83 | AAAA | C |
| ATOH | 1248 | O | ASP | 126 | 26.740 | 6.400 | 69.888 | 1.00 | 42.78 | AAAA | O |
| ATOH | 1249 | H | TRP | 127 | 26.029 | 6.649 | 67.704 | 1.00 | 35.42 | AAAA | H |
| ATOH | 1251 | CA | TRP | 127 | 26.777 | 7.856 | 67.410 | 1.00 | 33.02 | AAAA | C |
| ATOH | 1252 | CB | TRP | 127 | 26.568 | 8.296 | 65.930 | 1.00 | 24.89 | AAAA | C |
| ATOH | 1253 | CG | TRP | 127 | 27.195 | 7.372 | 64.907 | 1.00 | 34.36 | AAAA | C |
| ATOH | 1254 | CD2 | TRP | 127 | 28.587 | 7.208 | 64.518 | 1.00 | 28.60 | AAAA | C |
| ATOH | 1255 | CE2 | TRP | 127 | 28.631 | 6.186 | 63.579 | 1.00 | 29.06 | AAAA | C |
| ATOH | 1256 | CE3 | TRP | 127 | 29.778 | 7.845 | 64.873 | 1.00 | 35.51 | AAAA | C |
| ATOH | 1257 | CD1 | TRP | 127 | 26.465 | 6.450 | 64.188 | 1.00 | 18.67 | AAAA | C |
| ATOH | 1258 | HE1 | TRP | 127 | 27.311 | 5.712 | 63.394 | 1.00 | 42.87 | AAAA | H |
| ATOH | 1260 | CE2 | TRP | 127 | 29.792 | 5.783 | 62.954 | 1.00 | 32.53 | AAAA | C |
| ATOH | 1261 | CG3 | TRP | 127 | 30.972 | 7.445 | 64.285 | 1.00 | 31.51 | AAAA | C |
| ATOH | 1262 | CH2 | TRP | 127 | 30.937 | 6.405 | 63.336 | 1.00 | 37.86 | AAAA | C |
| ATOH | 1263 | C | TRP | 127 | 26.558 | 9.010 | 68.367 | 1.00 | 36.09 | AAAA | C |
| ATOH | 1264 | O | TRP | 127 | 27.382 | 9.977 | 68.497 | 1.00 | 40.87 | AAAA | O |
| ATOH | 1265 | H | SER | 128 | 25.493 | 8.931 | 69.171 | 1.00 | 31.24 | AAAA | H |
| ATOH | 1267 | CA | SER | 128 | 25.201 | 10.041 | 70.081 | 1.00 | 34.04 | AAAA | C |
| ATOH | 1268 | CB | SER | 128 | 23.757 | 10.042 | 70.603 | 1.00 | 36.87 | AAAA | C |
| ATOH | 1269 | CG | SER | 128 | 23.433 | 8.917 | 71.424 | 1.00 | 28.96 | AAAA | O |
| ATOH | 1271 | C | SER | 128 | 26.133 | 9.975 | 71.292 | 1.00 | 32.39 | AAAA | C |
| ATOH | 1272 | O | SER | 128 | 26.212 | 10.857 | 72.134 | 1.00 | 30.91 | AAAA | O |
| ATOH | 1273 | H | LEU | 129 | 26.662 | 8.792 | 71.549 | 1.00 | 27.18 | AAAA | H |
| ATOH | 1275 | CA | LEU | 129 | 27.701 | 8.607 | 72.526 | 1.00 | 36.73 | AAAA | C |
| ATOH | 1276 | CB | LEU | 129 | 27.920 | 7.132 | 72.741 | 1.00 | 32.53 | AAAA | C |
| ATOH | 1277 | CG | LEU | 129 | 26.795 | 6.324 | 73.371 | 1.00 | 39.28 | AAAA | C |
| ATOH | 1279 | CD1 | LEU | 129 | 27.292 | 5.024 | 73.975 | 1.00 | 32.54 | AAAA | C |
| ATOH | 1279 | CD2 | LEU | 129 | 26.237 | 7.117 | 74.560 | 1.00 | 32.12 | AAAA | C |
| ATOH | 1280 | C | LEU | 129 | 29.054 | 9.226 | 72.113 | 1.00 | 38.04 | AAAA | C |
| ATOH | 1281 | O | LEU | 129 | 29.645 | 10.001 | 72.874 | 1.00 | 34.50 | AAAA | O |
| ATOH | 1282 | H | ILE | 130 | 29.316 | 9.217 | 70.907 | 1.00 | 42.09 | AAAA | H |
| ATOH | 1284 | CA | ILE | 130 | 30.490 | 9.743 | 70.144 | 1.00 | 41.35 | AAAA | C |
| ATOH | 1285 | CB | ILE | 130 | 30.793 | 9.896 | 68.901 | 1.00 | 41.73 | AAAA | C |
| ATOH | 1286 | CG2 | ILE | 130 | 31.992 | 9.434 | 68.176 | 1.00 | 31.95 | AAAA | C |
| ATOH | 1287 | CG1 | ILE | 130 | 30.969 | 7.413 | 69.347 | 1.00 | 26.64 | AAAA | C |
| ATOH | 1288 | CD1 | ILE | 130 | 31.053 | 6.457 | 69.165 | 1.00 | 42.63 | AAAA | C |
| ATOH | 1289 | C | ILE | 130 | 30.305 | 11.178 | 69.679 | 1.00 | 46.48 | AAAA | C |
| ATOH | 1290 | O | ILE | 130 | 31.224 | 11.995 | 69.966 | 1.00 | 38.46 | AAAA | O |
| ATOH | 1291 | H | LEU | 131 | 29.089 | 11.495 | 69.193 | 1.00 | 45.14 | AAAA | H |
| ATOH | 1293 | CA | LEU | 131 | 29.895 | 12.965 | 68.651 | 1.00 | 41.45 | AAAA | C |
| ATOH | 1294 | CB | LEU | 131 | 28.499 | 12.616 | 67.259 | 1.00 | 46.81 | AAAA | C |
| ATOH | 1295 | CG | LEU | 131 | 29.823 | 12.905 | 65.878 | 1.00 | 36.79 | AAAA | C |
| ATOH | 1296 | CD1 | LEU | 131 | 29.128 | 11.405 | 65.324 | 1.00 | 30.15 | AAAA | C |
| ATOH | 1297 | CD2 | LEU | 131 | 27.625 | 13.581 | 65.334 | 1.00 | 19.92 | AAAA | C |
| ATOH | 1299 | C | LEU | 131 | 27.661 | 13.525 | 69.295 | 1.00 | 39.29 | AAAA | C |
| ATOH | 1299 | O | LEU | 131 | 26.599 | 12.967 | 69.311 | 1.00 | 37.75 | AAAA | O |
| ATOH | 1300 | H | ASP | 132 | 27.742 | 14.811 | 69.518 | 1.00 | 33.73 | AAAA | H |
| ATOH | 1302 | CA | ASP | 132 | 26.610 | 15.542 | 70.003 | 1.00 | 38.20 | AAAA | C |
| ATOH | 1303 | CB | ASP | 132 | 27.017 | 16.944 | 70.381 | 1.00 | 43.17 | AAAA | C |
| ATOH | 1304 | CG | ASP | 132 | 27.349 | 17.137 | 71.834 | 1.00 | 43.29 | AAAA | C |
| ATOH | 1305 | OD1 | ASP | 132 | 27.536 | 16.122 | 72.521 | 1.00 | 47.12 | AAAA | O |
| ATOH | 1306 | OD2 | ASP | 132 | 27.413 | 18.331 | 72.208 | 1.00 | 60.58 | AAAA | O |
| ATOH | 1307 | C | ASP | 132 | 25.520 | 15.659 | 68.946 | 1.00 | 43.46 | AAAA | C |
| ATOH | 1308 | O | ASP | 132 | 24.481 | 15.032 | 68.939 | 1.00 | 49.32 | AAAA | O |
| ATOH | 1309 | H | ALA | 133 | 25.754 | 16.398 | 67.900 | 1.00 | 45.03 | AAAA | H |
| ATOH | 1311 | CA | ALA | 133 | 24.947 | 16.776 | 66.773 | 1.00 | 38.62 | AAAA | C |
| ATOH | 1312 | CB | ALA | 133 | 25.628 | 17.987 | 66.092 | 1.00 | 33.92 | AAAA | C |
| ATOH | 1313 | C | ALA | 133 | 24.694 | 15.669 | 65.775 | 1.00 | 33.33 | AAAA | C |
| ATOH | 1314 | O | ALA | 133 | 24.777 | 15.791 | 64.517 | 1.00 | 33.71 | AAAA | O |
| ATOH | 1315 | H | VAL | 134 | 24.115 | 14.565 | 66.219 | 1.00 | 27.89 | AAAA | H |
| ATOH | 1317 | CA | VAL | 134 | 23.813 | 13.440 | 65.377 | 1.00 | 29.90 | AAAA | C |
| ATOH | 1318 | CB | VAL | 134 | 23.202 | 12.241 | 66.120 | 1.00 | 40.63 | AAAA | C |
| ATOH | 1319 | CG1 | VAL | 134 | 24.265 | 11.441 | 66.855 | 1.00 | 35.20 | AAAA | C |
| ATOH | 1320 | CG2 | VAL | 134 | 22.095 | 12.701 | 67.068 | 1.00 | 30.94 | AAAA | C |
| ATOH | 1321 | C | VAL | 134 | 22.735 | 13.732 | 64.353 | 1.00 | 36.99 | AAAA | C |
| ATOH | 1322 | O | VAL | 134 | 22.616 | 13.106 | 63.292 | 1.00 | 32.95 | AAAA | O |
| ATOH | 1323 | H | SER | 135 | 21.920 | 14.777 | 64.626 | 1.00 | 39.65 | AAAA | H |
| ATOH | 1325 | CA | SER | 135 | 20.886 | 15.139 | 63.692 | 1.00 | 43.12 | AAAA | C |
| ATOH | 1326 | CB | SER | 135 | 20.093 | 16.277 | 64.305 | 1.00 | 45.19 | AAAA | C |
| ATOH | 1327 | CG | SER | 135 | 20.882 | 17.369 | 64.684 | 1.00 | 39.25 | AAAA | O |
| ATOH | 1329 | C | SER | 135 | 21.396 | 15.516 | 62.309 | 1.00 | 41.15 | AAAA | C |
| ATOH | 1330 | O | SER | 135 | 20.615 | 15.642 | 61.359 | 1.00 | 43.81 | AAAA | O |
| ATOH | 1331 | H | ASN | 136 | 22.615 | 15.911 | 62.165 | 1.00 | 41.11 | AAAA | H |
| ATOH | 1333 | CA | ASN | 136 | 23.298 | 16.353 | 60.978 | 1.00 | 37.21 | AAAA | C |
| ATOH | 1334 | CB | ASN | 136 | 24.324 | 17.372 | 61.399 | 1.00 | 39.66 | AAAA | C |
| ATOH | 1335 | CG | ASN | 136 | 23.724 | 18.709 | 61.717 | 1.00 | 36.59 | AAAA | C |
| ATOH | 1336 | OD1 | ASN | 136 | 22.695 | 19.079 | 61.149 | 1.00 | 50.81 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 1337 | HD2 | ASN | 136 | 24.379 | 19.441 | 62.585 | 1.00 | 47.85 | AAAA | H |
| ATOM | 1340 | C | ASN | 136 | 24.031 | 15.230 | 60.259 | 1.00 | 35.31 | AAAA | C |
| ATOM | 1341 | O | ASN | 136 | 24.535 | 15.484 | 59.194 | 1.00 | 38.70 | AAAA | O |
| ATOM | 1342 | H | ASN | 137 | 24.057 | 14.035 | 60.793 | 1.00 | 29.11 | AAAA | H |
| ATOM | 1344 | CA | ASN | 137 | 24.721 | 12.959 | 60.126 | 1.00 | 32.98 | AAAA | C |
| ATOM | 1345 | CB | ASN | 137 | 24.737 | 11.703 | 61.033 | 1.00 | 24.45 | AAAA | C |
| ATOM | 1346 | CG | ASN | 137 | 25.631 | 11.965 | 62.217 | 1.00 | 26.63 | AAAA | C |
| ATOM | 1347 | OD1 | ASN | 137 | 26.070 | 13.121 | 62.369 | 1.00 | 30.22 | AAAA | O |
| ATOM | 1348 | HD2 | ASN | 137 | 25.830 | 10.923 | 63.000 | 1.00 | 18.90 | AAAA | H |
| ATOM | 1351 | C | ASN | 137 | 23.950 | 12.749 | 58.817 | 1.00 | 35.89 | AAAA | C |
| ATOM | 1352 | O | ASN | 137 | 22.716 | 12.755 | 58.855 | 1.00 | 38.57 | AAAA | O |
| ATOM | 1353 | H | TYR | 138 | 24.592 | 12.251 | 57.785 | 1.00 | 32.86 | AAAA | H |
| ATOM | 1355 | CA | TYR | 138 | 24.093 | 11.983 | 56.489 | 1.00 | 30.25 | AAAA | C |
| ATOM | 1356 | CB | TYR | 138 | 24.682 | 12.861 | 55.421 | 1.00 | 27.10 | AAAA | C |
| ATOM | 1357 | CG | TYR | 138 | 24.018 | 12.741 | 54.079 | 1.00 | 37.89 | AAAA | C |
| ATOM | 1358 | CD1 | TYR | 138 | 23.083 | 13.671 | 53.648 | 1.00 | 39.22 | AAAA | C |
| ATOM | 1359 | CE1 | TYR | 138 | 22.510 | 13.579 | 52.392 | 1.00 | 37.65 | AAAA | C |
| ATOM | 1360 | CD2 | TYR | 138 | 24.357 | 11.717 | 53.195 | 1.00 | 44.28 | AAAA | C |
| ATOM | 1361 | CE2 | TYR | 138 | 23.801 | 11.615 | 51.951 | 1.00 | 41.97 | AAAA | C |
| ATOM | 1362 | CG | TYR | 138 | 22.868 | 12.562 | 51.564 | 1.00 | 39.42 | AAAA | C |
| ATOM | 1363 | OH | TYR | 138 | 22.296 | 12.504 | 50.318 | 1.00 | 45.48 | AAAA | O |
| ATOM | 1365 | C | TYR | 138 | 24.373 | 10.578 | 56.051 | 1.00 | 31.33 | AAAA | C |
| ATOM | 1366 | O | TYR | 138 | 25.505 | 10.317 | 55.797 | 1.00 | 37.76 | AAAA | O |
| ATOM | 1367 | H | ILE | 139 | 23.461 | 9.660 | 56.116 | 1.00 | 35.40 | AAAA | H |
| ATOM | 1369 | CA | ILE | 139 | 23.637 | 8.249 | 55.935 | 1.00 | 34.04 | AAAA | C |
| ATOM | 1370 | CB | ILE | 139 | 23.234 | 7.450 | 57.171 | 1.00 | 28.66 | AAAA | C |
| ATOM | 1371 | CG2 | ILE | 139 | 23.640 | 5.984 | 57.093 | 1.00 | 21.99 | AAAA | C |
| ATOM | 1372 | CG1 | ILE | 139 | 23.711 | 8.057 | 58.469 | 1.00 | 42.81 | AAAA | C |
| ATOM | 1373 | CD1 | ILE | 139 | 24.455 | 7.100 | 59.389 | 1.00 | 52.23 | AAAA | C |
| ATOM | 1374 | C | ILE | 139 | 22.729 | 7.708 | 54.830 | 1.00 | 35.73 | AAAA | C |
| ATOM | 1375 | O | ILE | 139 | 21.538 | 7.890 | 54.757 | 1.00 | 42.61 | AAAA | O |
| ATOM | 1376 | H | VAL | 140 | 23.286 | 6.997 | 53.873 | 1.00 | 35.29 | AAAA | H |
| ATOM | 1378 | CA | VAL | 140 | 22.533 | 6.481 | 52.755 | 1.00 | 32.39 | AAAA | C |
| ATOM | 1379 | CB | VAL | 140 | 21.967 | 7.627 | 51.981 | 1.00 | 36.05 | AAAA | C |
| ATOM | 1380 | CG1 | VAL | 140 | 22.800 | 8.375 | 50.881 | 1.00 | 25.89 | AAAA | C |
| ATOM | 1381 | CG2 | VAL | 140 | 20.807 | 7.034 | 51.047 | 1.00 | 34.96 | AAAA | C |
| ATOM | 1382 | O | VAL | 140 | 23.422 | 5.670 | 51.874 | 1.00 | 41.96 | AAAA | O |
| ATOM | 1383 | C | VAL | 140 | 24.537 | 6.172 | 51.637 | 1.00 | 44.03 | AAAA | C |
| ATOM | 1384 | H | GLY | 141 | 22.899 | 4.562 | 51.402 | 1.00 | 42.66 | AAAA | H |
| ATOM | 1386 | CA | GLY | 141 | 23.361 | 3.805 | 50.279 | 1.00 | 30.94 | AAAA | C |
| ATOM | 1387 | C | GLY | 141 | 24.265 | 2.696 | 50.935 | 1.00 | 38.99 | AAAA | C |
| ATOM | 1388 | O | GLY | 141 | 25.132 | 2.003 | 50.176 | 1.00 | 35.87 | AAAA | O |
| ATOM | 1389 | H | ASN | 142 | 23.985 | 2.418 | 52.116 | 1.00 | 38.92 | AAAA | H |
| ATOM | 1391 | CA | ASN | 142 | 24.958 | 1.390 | 52.746 | 1.00 | 44.32 | AAAA | C |
| ATOM | 1392 | CB | ASN | 142 | 25.257 | 1.774 | 54.187 | 1.00 | 43.12 | AAAA | C |
| ATOM | 1393 | CG | ASN | 142 | 26.131 | 3.022 | 54.152 | 1.00 | 42.00 | AAAA | C |
| ATOM | 1394 | OD1 | ASN | 142 | 26.984 | 3.077 | 53.269 | 1.00 | 40.47 | AAAA | O |
| ATOM | 1395 | HD2 | ASN | 142 | 25.945 | 4.022 | 55.219 | 1.00 | 41.99 | AAAA | H |
| ATOM | 1398 | C | ASN | 142 | 24.153 | 0.066 | 52.687 | 1.00 | 45.84 | AAAA | C |
| ATOM | 1399 | O | ASN | 142 | 23.113 | -0.015 | 52.055 | 1.00 | 49.65 | AAAA | O |
| ATOM | 1400 | H | LYS | 143 | 24.674 | -0.990 | 53.272 | 1.00 | 45.23 | AAAA | H |
| ATOM | 1402 | CA | LYS | 143 | 24.073 | -2.299 | 53.195 | 1.00 | 49.14 | AAAA | C |
| ATOM | 1403 | CB | LYS | 143 | 25.166 | -3.328 | 53.433 | 1.00 | 41.49 | AAAA | C |
| ATOM | 1404 | CG | LYS | 143 | 24.750 | -4.686 | 53.832 | 1.00 | 44.96 | AAAA | C |
| ATOM | 1405 | CD | LYS | 143 | 25.512 | -5.743 | 53.100 | 1.00 | 48.66 | AAAA | C |
| ATOM | 1406 | CE | LYS | 143 | 25.043 | -7.131 | 53.558 | 1.00 | 38.35 | AAAA | C |
| ATOM | 1407 | HD | LYS | 143 | 26.080 | -8.093 | 53.040 | 1.00 | 53.83 | AAAA | H |
| ATOM | 1411 | C | LYS | 143 | 22.902 | -2.431 | 54.169 | 1.00 | 52.85 | AAAA | C |
| ATOM | 1412 | O | LYS | 143 | 22.960 | -2.099 | 55.360 | 1.00 | 55.21 | AAAA | O |
| ATOM | 1413 | H | PRO | 144 | 21.806 | -3.047 | 53.731 | 1.00 | 52.39 | AAAA | H |
| ATOM | 1414 | CD | PRO | 144 | 21.617 | -3.469 | 52.315 | 1.00 | 52.58 | AAAA | C |
| ATOM | 1415 | CA | PRO | 144 | 20.559 | -3.118 | 54.489 | 1.00 | 49.30 | AAAA | C |
| ATOM | 1416 | CB | PRO | 144 | 19.549 | -3.602 | 53.455 | 1.00 | 51.41 | AAAA | C |
| ATOM | 1417 | CG | PRO | 144 | 20.134 | -3.299 | 52.099 | 1.00 | 50.41 | AAAA | C |
| ATOM | 1418 | C | PRO | 144 | 20.621 | -4.050 | 55.659 | 1.00 | 44.65 | AAAA | C |
| ATOM | 1419 | O | PRO | 144 | 20.904 | -5.236 | 55.501 | 1.00 | 36.84 | AAAA | O |
| ATOM | 1420 | H | PRO | 145 | 20.318 | -3.533 | 56.859 | 1.00 | 45.12 | AAAA | H |
| ATOM | 1421 | CD | PRO | 145 | 20.123 | -2.054 | 57.094 | 1.00 | 38.17 | AAAA | C |
| ATOM | 1422 | CA | PRO | 145 | 20.448 | -4.233 | 58.128 | 1.00 | 40.19 | AAAA | C |
| ATOM | 1423 | CB | PRO | 145 | 19.704 | -3.288 | 59.099 | 1.00 | 37.08 | AAAA | C |
| ATOM | 1424 | CG | PRO | 145 | 20.040 | -1.910 | 58.602 | 1.00 | 33.65 | AAAA | C |
| ATOM | 1425 | C | PRO | 145 | 19.993 | -5.655 | 58.155 | 1.00 | 47.17 | AAAA | C |
| ATOM | 1426 | O | PRO | 145 | 20.556 | -6.592 | 58.768 | 1.00 | 49.05 | AAAA | O |
| ATOM | 1427 | H | LYS | 146 | 18.879 | -5.924 | 57.499 | 1.00 | 53.72 | AAAA | H |
| ATOM | 1429 | CA | LYS | 146 | 18.268 | -7.229 | 57.295 | 1.00 | 56.94 | AAAA | C |
| ATOM | 1430 | CB | LYS | 146 | 16.894 | -7.050 | 56.647 | 1.00 | 65.44 | AAAA | C |
| ATOM | 1431 | CG | LYS | 146 | 16.220 | -8.232 | 55.982 | 1.00 | 64.32 | AAAA | C |
| ATOM | 1432 | CD | LYS | 146 | 14.797 | -8.422 | 56.451 | 0.01 | 62.75 | AAAA | C |
| ATOM | 1433 | CE | LYS | 146 | 14.194 | -9.717 | 55.934 | 0.01 | 62.14 | AAAA | C |
| ATOM | 1434 | HD | LYS | 146 | 12.720 | -9.610 | 55.753 | 0.01 | 61.38 | AAAA | H |
| ATOM | 1438 | C | LYS | 146 | 19.138 | -8.138 | 56.446 | 1.00 | 61.40 | AAAA | C |
| ATOM | 1439 | O | LYS | 146 | 19.237 | -9.346 | 56.732 | 1.00 | 66.22 | AAAA | O |
| ATOM | 1440 | H | GLU | 147 | 19.779 | -7.649 | 55.389 | 1.00 | 62.92 | AAAA | H |
| ATOM | 1442 | CA | GLU | 147 | 20.827 | -8.446 | 54.742 | 1.00 | 67.00 | AAAA | C |
| ATOM | 1443 | CB | GLU | 147 | 21.101 | -8.070 | 53.294 | 1.00 | 62.32 | AAAA | C |

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|------|------|-----|-----|-----|--------|---------|--------|------|--------|------|---|
| ATOM | 1444 | U1 | GLU | 147 | 19.367 | -7.579 | 52.567 | 1.00 | 73.15 | AAAA | C |
| ATOM | 1445 | CD | GLU | 147 | 20.164 | -7.413 | 51.093 | 1.00 | 85.90 | AAAA | C |
| ATOM | 1446 | OE1 | GLU | 147 | 21.339 | -7.636 | 50.701 | 1.00 | 95.25 | AAAA | O |
| ATOM | 1447 | OE2 | GLU | 147 | 19.201 | -7.053 | 50.376 | 1.00 | 87.47 | AAAA | O |
| ATOM | 1448 | C | GLU | 147 | 22.136 | -8.470 | 55.541 | 1.00 | 69.40 | AAAA | C |
| ATOM | 1449 | O | GLU | 147 | 22.883 | -9.437 | 55.361 | 1.00 | 72.86 | AAAA | O |
| ATOM | 1450 | H | CYS | 148 | 22.506 | -7.484 | 56.355 | 1.00 | 66.76 | AAAA | H |
| ATOM | 1451 | CA | CYS | 148 | 23.693 | -7.588 | 57.183 | 1.00 | 64.65 | AAAA | C |
| ATOM | 1452 | C | CYS | 148 | 23.598 | -8.702 | 58.196 | 1.00 | 65.56 | AAAA | C |
| ATOM | 1453 | O | CYS | 148 | 24.473 | -9.524 | 58.414 | 1.00 | 65.89 | AAAA | O |
| ATOM | 1454 | CB | CYS | 148 | 23.952 | -6.301 | 58.001 | 1.00 | 57.29 | AAAA | C |
| ATOM | 1455 | SG | CYS | 148 | 24.565 | -5.091 | 56.808 | 1.00 | 59.22 | AAAA | S |
| ATOM | 1456 | H | GLY | 149 | 22.514 | -8.743 | 58.977 | 1.00 | 67.88 | AAAA | H |
| ATOM | 1457 | CA | GLY | 149 | 22.387 | -9.744 | 60.029 | 1.00 | 62.15 | AAAA | C |
| ATOM | 1458 | C | GLY | 149 | 23.443 | -9.627 | 61.120 | 1.00 | 59.18 | AAAA | C |
| ATOM | 1459 | O | GLY | 149 | 23.925 | -10.603 | 61.699 | 1.00 | 61.11 | AAAA | O |
| ATOM | 1460 | H | ASP | 150 | 23.717 | -8.426 | 61.596 | 1.00 | 54.88 | AAAA | H |
| ATOM | 1461 | CA | ASP | 150 | 24.794 | -8.198 | 62.533 | 1.00 | 55.78 | AAAA | C |
| ATOM | 1462 | CB | ASP | 150 | 25.041 | -6.703 | 62.750 | 1.00 | 49.10 | AAAA | C |
| ATOM | 1463 | CG | ASP | 150 | 25.320 | -6.034 | 61.410 | 1.00 | 58.50 | AAAA | C |
| ATOM | 1464 | OD1 | ASP | 150 | 25.726 | -6.796 | 60.480 | 1.00 | 57.73 | AAAA | O |
| ATOM | 1465 | OD2 | ASP | 150 | 25.102 | -4.819 | 61.363 | 1.00 | 49.69 | AAAA | O |
| ATOM | 1466 | C | ASP | 150 | 24.519 | -9.854 | 63.855 | 1.00 | 59.36 | AAAA | C |
| ATOM | 1467 | O | ASP | 150 | 23.392 | -8.820 | 64.377 | 1.00 | 67.48 | AAAA | O |
| ATOM | 1471 | H | LEU | 151 | 25.532 | -9.369 | 64.524 | 1.00 | 54.39 | AAAA | H |
| ATOM | 1472 | CA | LEU | 151 | 25.314 | -9.908 | 65.853 | 1.00 | 52.79 | AAAA | C |
| ATOM | 1473 | CB | LEU | 151 | 25.208 | -11.409 | 65.806 | 1.00 | 58.55 | AAAA | C |
| ATOM | 1474 | CG | LEU | 151 | 24.063 | -12.101 | 65.092 | 1.00 | 69.45 | AAAA | C |
| ATOM | 1475 | CD1 | LEU | 151 | 24.515 | -13.421 | 64.489 | 1.00 | 65.26 | AAAA | C |
| ATOM | 1476 | CD2 | LEU | 151 | 22.837 | -12.372 | 65.951 | 1.00 | 65.43 | AAAA | C |
| ATOM | 1477 | C | LEU | 151 | 26.409 | -9.454 | 66.805 | 1.00 | 51.93 | AAAA | C |
| ATOM | 1478 | O | LEU | 151 | 27.598 | -9.734 | 66.634 | 1.00 | 55.59 | AAAA | O |
| ATOM | 1479 | H | CYS | 152 | 26.024 | -8.773 | 67.849 | 1.00 | 48.62 | AAAA | H |
| ATOM | 1480 | CA | CYS | 152 | 26.992 | -9.189 | 68.740 | 1.00 | 56.73 | AAAA | C |
| ATOM | 1481 | C | CYS | 152 | 27.650 | -9.325 | 69.493 | 1.00 | 63.58 | AAAA | C |
| ATOM | 1482 | O | CYS | 152 | 27.074 | -10.405 | 69.575 | 1.00 | 62.40 | AAAA | O |
| ATOM | 1483 | CB | CYS | 152 | 26.358 | -7.144 | 69.657 | 1.00 | 41.99 | AAAA | C |
| ATOM | 1484 | CG | CYS | 152 | 25.935 | -5.635 | 68.703 | 1.00 | 55.93 | AAAA | S |
| ATOM | 1485 | H | PRO | 153 | 29.825 | -9.072 | 70.059 | 1.00 | 68.05 | AAAA | H |
| ATOM | 1486 | CD | PRO | 153 | 29.618 | -7.838 | 69.903 | 1.00 | 66.66 | AAAA | C |
| ATOM | 1487 | CA | PRO | 153 | 29.497 | -10.094 | 70.851 | 1.00 | 70.60 | AAAA | C |
| ATOM | 1488 | CB | PRO | 153 | 30.601 | -9.323 | 71.557 | 1.00 | 69.98 | AAAA | C |
| ATOM | 1489 | CG | PRO | 153 | 30.861 | -9.159 | 70.690 | 1.00 | 70.58 | AAAA | C |
| ATOM | 1490 | C | PRO | 153 | 29.543 | -10.734 | 71.850 | 1.00 | 69.64 | AAAA | C |
| ATOM | 1491 | O | PRO | 153 | 27.959 | -10.075 | 72.615 | 1.00 | 69.58 | AAAA | O |
| ATOM | 1492 | H | GLY | 154 | 28.444 | -12.049 | 71.943 | 1.00 | 71.23 | AAAA | H |
| ATOM | 1493 | CA | GLY | 154 | 27.610 | -12.904 | 72.745 | 1.00 | 78.07 | AAAA | C |
| ATOM | 1494 | C | GLY | 154 | 26.245 | -13.230 | 72.223 | 1.00 | 81.75 | AAAA | C |
| ATOM | 1495 | O | GLY | 154 | 25.736 | -14.318 | 72.547 | 1.00 | 80.26 | AAAA | O |
| ATOM | 1496 | H | THR | 155 | 25.649 | -10.468 | 71.314 | 1.00 | 84.54 | AAAA | H |
| ATOM | 1501 | CA | THR | 155 | 24.314 | -10.683 | 70.828 | 1.00 | 89.38 | AAAA | C |
| ATOM | 1502 | CB | THR | 155 | 24.016 | -11.661 | 69.705 | 1.00 | 85.07 | AAAA | C |
| ATOM | 1503 | CG1 | THR | 155 | 24.063 | -10.417 | 70.420 | 1.00 | 84.51 | AAAA | O |
| ATOM | 1504 | CG2 | THR | 155 | 22.686 | -11.995 | 69.092 | 1.00 | 82.27 | AAAA | C |
| ATOM | 1505 | C | THR | 155 | 24.060 | -14.094 | 70.353 | 1.00 | 93.69 | AAAA | C |
| ATOM | 1506 | O | THR | 155 | 23.005 | -14.664 | 70.617 | 1.00 | 95.92 | AAAA | O |
| ATOM | 1508 | H | NET | 156 | 25.003 | -14.655 | 69.617 | 1.00 | 97.23 | AAAA | H |
| ATOM | 1510 | CA | NET | 156 | 24.884 | -15.973 | 69.024 | 1.00 | 99.05 | AAAA | C |
| ATOM | 1511 | CB | NET | 156 | 25.907 | -16.190 | 67.896 | 1.00 | 100.40 | AAAA | C |
| ATOM | 1512 | CG | NET | 156 | 25.456 | -15.675 | 66.542 | 0.01 | 99.75 | AAAA | C |
| ATOM | 1513 | SD | NET | 156 | 23.637 | -15.857 | 66.255 | 0.01 | 99.72 | AAAA | S |
| ATOM | 1514 | CE | NET | 156 | 23.664 | -17.214 | 65.087 | 0.01 | 99.59 | AAAA | C |
| ATOM | 1515 | C | NET | 156 | 25.027 | -17.106 | 70.032 | 1.00 | 100.57 | AAAA | C |
| ATOM | 1516 | O | NET | 156 | 24.353 | -18.122 | 69.835 | 1.00 | 101.64 | AAAA | O |
| ATOM | 1517 | H | ALA | 157 | 25.974 | -17.057 | 70.967 | 1.00 | 100.53 | AAAA | H |
| ATOM | 1519 | CA | ALA | 157 | 26.022 | -18.102 | 71.986 | 1.00 | 101.00 | AAAA | C |
| ATOM | 1520 | CB | ALA | 157 | 27.317 | -19.158 | 72.766 | 1.00 | 103.42 | AAAA | C |
| ATOM | 1521 | C | ALA | 157 | 24.856 | -17.890 | 72.959 | 1.00 | 101.10 | AAAA | C |
| ATOM | 1522 | O | ALA | 157 | 23.893 | -18.654 | 72.921 | 1.00 | 104.59 | AAAA | O |
| ATOM | 1523 | H | GLU | 158 | 24.984 | -16.906 | 73.841 | 1.00 | 98.39 | AAAA | H |
| ATOM | 1524 | CA | GLU | 158 | 23.935 | -16.629 | 74.781 | 1.00 | 97.43 | AAAA | C |
| ATOM | 1525 | CB | GLU | 158 | 23.128 | -17.965 | 75.208 | 1.00 | 105.93 | AAAA | C |
| ATOM | 1526 | CG | GLU | 158 | 21.687 | -17.546 | 75.560 | 1.00 | 113.87 | AAAA | C |
| ATOM | 1527 | CD | GLU | 158 | 21.347 | -16.081 | 75.302 | 1.00 | 119.34 | AAAA | C |
| ATOM | 1528 | OE1 | GLU | 159 | 21.284 | -15.733 | 74.096 | 1.00 | 126.27 | AAAA | O |
| ATOM | 1529 | OE2 | GLU | 158 | 21.199 | -15.317 | 76.282 | 1.00 | 117.79 | AAAA | O |
| ATOM | 1531 | C | GLU | 158 | 24.434 | -15.915 | 76.025 | 1.00 | 95.00 | AAAA | C |
| ATOM | 1532 | O | GLU | 158 | 23.988 | -16.117 | 77.145 | 1.00 | 95.89 | AAAA | O |
| ATOM | 1533 | H | SER | 159 | 25.276 | -14.942 | 75.769 | 1.00 | 93.30 | AAAA | H |
| ATOM | 1534 | CA | SER | 159 | 25.810 | -14.119 | 76.848 | 1.00 | 92.28 | AAAA | C |
| ATOM | 1535 | CB | SER | 159 | 26.989 | -14.905 | 77.517 | 1.00 | 97.37 | AAAA | C |
| ATOM | 1536 | CG | SER | 159 | 26.972 | -14.427 | 78.886 | 1.00 | 98.08 | AAAA | O |
| ATOM | 1537 | C | SER | 159 | 26.228 | -12.793 | 76.226 | 1.00 | 91.47 | AAAA | C |
| ATOM | 1538 | O | SER | 159 | 27.368 | -12.532 | 75.810 | 1.00 | 92.75 | AAAA | O |
| ATOM | 1540 | H | PRO | 160 | 25.196 | -12.007 | 75.932 | 1.00 | 88.65 | AAAA | H |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|---|
| ATOM | 1542 | CU | PRO | 160 | 23.789 | -12.122 | 76.395 | 1.00 | 86.67 | AAAA | C |
| ATOM | 1543 | CA | PRO | 160 | 25.463 | -10.701 | 75.361 | 1.00 | 84.74 | AAAA | C |
| ATOM | 1544 | CB | PRO | 160 | 24.125 | -9.978 | 75.456 | 1.00 | 84.79 | AAAA | C |
| ATOM | 1545 | CG | PRO | 160 | 23.370 | -10.671 | 76.515 | 1.00 | 84.62 | AAAA | C |
| ATOM | 1546 | C | PRO | 160 | 26.503 | -10.025 | 76.236 | 1.00 | 79.60 | AAAA | C |
| ATOM | 1547 | O | PRO | 160 | 26.319 | -9.934 | 77.456 | 1.00 | 79.70 | AAAA | O |
| ATOM | 1548 | H | MET | 161 | 27.563 | -9.522 | 75.596 | 1.00 | 74.45 | AAAA | N |
| ATOM | 1550 | CA | MET | 161 | 28.530 | -8.735 | 76.378 | 1.00 | 67.04 | AAAA | C |
| ATOM | 1551 | CB | MET | 161 | 29.924 | -9.178 | 76.038 | 1.00 | 69.93 | AAAA | C |
| ATOM | 1552 | CG | MET | 161 | 30.118 | -10.630 | 75.706 | 1.00 | 71.43 | AAAA | C |
| ATOM | 1553 | SD | MET | 161 | 30.716 | -11.621 | 77.094 | 1.00 | 85.25 | AAAA | S |
| ATOM | 1554 | CE | MET | 161 | 29.841 | -10.905 | 78.471 | 1.00 | 69.31 | AAAA | C |
| ATOM | 1555 | C | MET | 161 | 28.358 | -7.234 | 76.189 | 1.00 | 61.76 | AAAA | C |
| ATOM | 1556 | O | MET | 161 | 28.788 | -6.443 | 77.034 | 1.00 | 58.60 | AAAA | O |
| ATOM | 1557 | H | CYS | 162 | 27.681 | -6.819 | 75.095 | 1.00 | 54.81 | AAAA | H |
| ATOM | 1559 | CA | CYS | 162 | 27.493 | -5.384 | 74.938 | 1.00 | 49.76 | AAAA | C |
| ATOM | 1560 | C | CYS | 162 | 26.306 | -4.777 | 75.670 | 1.00 | 51.52 | AAAA | C |
| ATOM | 1561 | O | CYS | 162 | 25.224 | -5.324 | 75.928 | 1.00 | 53.89 | AAAA | O |
| ATOM | 1562 | CB | CYS | 162 | 27.422 | -5.099 | 73.459 | 1.00 | 48.31 | AAAA | C |
| ATOM | 1563 | SG | CYS | 162 | 28.533 | -6.064 | 72.432 | 1.00 | 54.02 | AAAA | S |
| ATOM | 1564 | H | GLU | 163 | 26.409 | -3.522 | 76.031 | 1.00 | 46.31 | AAAA | H |
| ATOM | 1566 | CA | GLU | 163 | 25.355 | -2.675 | 76.538 | 1.00 | 47.19 | AAAA | C |
| ATOM | 1567 | CB | GLU | 163 | 26.051 | -1.412 | 77.027 | 1.00 | 49.95 | AAAA | C |
| ATOM | 1568 | CG | GLU | 163 | 26.476 | -1.364 | 78.465 | 1.00 | 62.30 | AAAA | C |
| ATOM | 1569 | CD | GLU | 163 | 25.817 | -0.135 | 79.116 | 1.00 | 81.67 | AAAA | C |
| ATOM | 1570 | OE1 | GLU | 163 | 26.470 | 0.473 | 80.016 | 1.00 | 73.22 | AAAA | O |
| ATOM | 1571 | OE2 | GLU | 163 | 24.646 | 0.208 | 78.721 | 1.00 | 80.93 | AAAA | O |
| ATOM | 1572 | C | GLU | 163 | 24.299 | -2.340 | 75.472 | 1.00 | 49.05 | AAAA | C |
| ATOM | 1573 | O | GLU | 163 | 24.488 | -2.423 | 74.234 | 1.00 | 45.90 | AAAA | O |
| ATOM | 1574 | H | LYS | 164 | 23.142 | -1.815 | 75.880 | 1.00 | 47.43 | AAAA | H |
| ATOM | 1576 | CA | LYS | 164 | 22.011 | -1.499 | 75.081 | 1.00 | 43.92 | AAAA | C |
| ATOM | 1577 | CB | LYS | 164 | 20.714 | -2.244 | 75.450 | 1.00 | 44.48 | AAAA | C |
| ATOM | 1578 | CG | LYS | 164 | 20.560 | -3.639 | 74.870 | 1.00 | 48.65 | AAAA | C |
| ATOM | 1579 | CD | LYS | 164 | 19.480 | -4.432 | 75.622 | 1.00 | 49.04 | AAAA | C |
| ATOM | 1580 | CE | LYS | 164 | 18.409 | -5.012 | 74.720 | 1.00 | 49.21 | AAAA | C |
| ATOM | 1581 | NC | LYS | 164 | 17.951 | -6.372 | 75.134 | 1.00 | 37.67 | AAAA | H |
| ATOM | 1585 | C | LYS | 164 | 21.615 | -0.040 | 75.204 | 1.00 | 45.01 | AAAA | C |
| ATOM | 1586 | O | LYS | 164 | 21.466 | 0.484 | 76.282 | 1.00 | 45.69 | AAAA | O |
| ATOM | 1587 | H | THR | 165 | 21.333 | 0.570 | 74.034 | 1.00 | 44.94 | AAAA | H |
| ATOM | 1589 | CA | THR | 165 | 20.775 | 1.943 | 74.077 | 1.00 | 43.13 | AAAA | C |
| ATOM | 1590 | CB | THR | 165 | 21.931 | 2.952 | 73.553 | 1.00 | 47.81 | AAAA | C |
| ATOM | 1591 | OE1 | THR | 165 | 22.053 | 2.689 | 72.127 | 1.00 | 39.13 | AAAA | O |
| ATOM | 1593 | CG2 | THR | 165 | 23.119 | 2.842 | 74.362 | 1.00 | 40.40 | AAAA | C |
| ATOM | 1594 | C | THR | 165 | 19.532 | 1.881 | 73.189 | 1.00 | 40.92 | AAAA | C |
| ATOM | 1598 | O | THR | 165 | 19.346 | 0.897 | 72.414 | 1.00 | 35.91 | AAAA | O |
| ATOM | 1596 | H | THR | 166 | 19.781 | 2.985 | 73.173 | 1.00 | 39.18 | AAAA | H |
| ATOM | 1599 | CA | THR | 166 | 17.689 | 3.991 | 72.182 | 1.00 | 42.97 | AAAA | C |
| ATOM | 1599 | CE | THR | 166 | 16.297 | 3.096 | 72.833 | 1.00 | 55.99 | AAAA | C |
| ATOM | 1600 | CG1 | THR | 166 | 15.662 | 4.385 | 72.819 | 1.00 | 41.42 | AAAA | O |
| ATOM | 1600 | CG2 | THR | 166 | 16.157 | 2.740 | 74.313 | 1.00 | 42.93 | AAAA | C |
| ATOM | 1603 | C | THR | 166 | 17.983 | 4.051 | 71.137 | 1.00 | 40.17 | AAAA | C |
| ATOM | 1604 | O | THR | 166 | 18.219 | 5.206 | 71.509 | 1.00 | 35.72 | AAAA | O |
| ATOM | 1605 | H | ILE | 167 | 17.912 | 3.725 | 69.866 | 1.00 | 42.21 | AAAA | H |
| ATOM | 1607 | CA | ILE | 167 | 18.182 | 4.672 | 68.777 | 1.00 | 41.05 | AAAA | C |
| ATOM | 1608 | CB | ILE | 167 | 19.437 | 4.335 | 67.904 | 1.00 | 39.50 | AAAA | C |
| ATOM | 1609 | CG2 | ILE | 167 | 19.589 | 5.346 | 66.716 | 1.00 | 15.26 | AAAA | C |
| ATOM | 1610 | CG1 | ILE | 167 | 20.722 | 4.305 | 68.724 | 1.00 | 36.20 | AAAA | C |
| ATOM | 1611 | CD1 | ILE | 167 | 21.899 | 3.665 | 67.966 | 1.00 | 35.70 | AAAA | C |
| ATOM | 1612 | C | ILE | 167 | 16.937 | 4.524 | 67.882 | 1.00 | 40.94 | AAAA | C |
| ATOM | 1613 | O | ILE | 167 | 16.655 | 3.435 | 67.394 | 1.00 | 35.51 | AAAA | O |
| ATOM | 1614 | H | ASN | 168 | 16.318 | 5.635 | 67.537 | 1.00 | 42.29 | AAAA | N |
| ATOM | 1616 | CA | ASN | 168 | 15.112 | 5.633 | 66.713 | 1.00 | 45.22 | AAAA | C |
| ATOM | 1617 | CB | ASN | 168 | 15.526 | 5.253 | 65.292 | 1.00 | 45.69 | AAAA | C |
| ATOM | 1618 | CG | ASN | 168 | 14.497 | 5.696 | 64.244 | 1.00 | 51.19 | AAAA | C |
| ATOM | 1619 | OD1 | ASN | 168 | 14.344 | 5.112 | 63.150 | 1.00 | 41.75 | AAAA | O |
| ATOM | 1620 | ND2 | ASN | 168 | 13.749 | 6.763 | 64.522 | 1.00 | 48.89 | AAAA | H |
| ATOM | 1623 | C | ASN | 168 | 13.954 | 4.739 | 67.141 | 1.00 | 46.55 | AAAA | C |
| ATOM | 1624 | O | ASN | 168 | 13.544 | 3.879 | 66.326 | 1.00 | 45.95 | AAAA | O |
| ATOM | 1625 | H | ASN | 169 | 13.644 | 4.728 | 68.433 | 1.00 | 45.12 | AAAA | H |
| ATOM | 1627 | CA | ASN | 169 | 12.717 | 3.759 | 69.007 | 1.00 | 43.67 | AAAA | C |
| ATOM | 1628 | CB | ASN | 169 | 11.315 | 4.106 | 68.540 | 1.00 | 36.84 | AAAA | C |
| ATOM | 1629 | CG | ASN | 169 | 10.943 | 5.487 | 69.093 | 1.00 | 42.75 | AAAA | C |
| ATOM | 1630 | OD1 | ASN | 169 | 10.917 | 5.779 | 70.280 | 1.00 | 36.67 | AAAA | O |
| ATOM | 1631 | ND2 | ASN | 169 | 10.659 | 6.449 | 68.213 | 1.00 | 40.74 | AAAA | H |
| ATOM | 1634 | C | ASN | 169 | 13.003 | 2.306 | 68.719 | 1.00 | 44.69 | AAAA | C |
| ATOM | 1635 | O | ASN | 169 | 12.100 | 1.544 | 68.383 | 1.00 | 45.72 | AAAA | O |
| ATOM | 1636 | H | GLU | 170 | 14.226 | 1.907 | 68.862 | 1.00 | 41.64 | AAAA | H |
| ATOM | 1638 | CA | GLU | 170 | 14.655 | 0.513 | 68.850 | 1.00 | 45.88 | AAAA | C |
| ATOM | 1639 | CB | GLU | 170 | 15.283 | 0.278 | 67.524 | 1.00 | 55.92 | AAAA | C |
| ATOM | 1640 | CG | GLU | 170 | 15.028 | -0.953 | 66.702 | 1.00 | 67.08 | AAAA | C |
| ATOM | 1641 | CD | GLU | 170 | 14.517 | -0.605 | 65.294 | 1.00 | 74.56 | AAAA | C |
| ATOM | 1642 | OE1 | GLU | 170 | 13.869 | 0.466 | 65.049 | 1.00 | 77.75 | AAAA | O |
| ATOM | 1643 | OE2 | GLU | 170 | 14.763 | -1.437 | 64.389 | 1.00 | 70.71 | AAAA | O |
| ATOM | 1644 | C | GLU | 170 | 15.647 | 0.379 | 70.010 | 1.00 | 47.10 | AAAA | C |
| ATOM | 1645 | O | GLU | 170 | 16.582 | 1.172 | 70.213 | 1.00 | 49.92 | AAAA | O |

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|------|------|-----|-----|-----|--------|---------|--------|------|-------|------|---|
| ATOH | 1646 | H | TYR | 171 | 15.344 | -0.462 | 70.952 | 1.00 | 49.10 | AAAA | H |
| ATOH | 1648 | CA | TYR | 171 | 16.231 | -0.688 | 72.097 | 1.00 | 51.81 | AAAA | C |
| ATOH | 1649 | CB | TYR | 171 | 15.434 | -0.861 | 73.359 | 1.00 | 49.94 | AAAA | C |
| ATOH | 1650 | CG | TYR | 171 | 16.175 | -1.168 | 74.620 | 1.00 | 48.90 | AAAA | C |
| ATOH | 1651 | CD1 | TYR | 171 | 16.980 | -0.210 | 75.237 | 1.00 | 46.46 | AAAA | C |
| ATOH | 1652 | CE1 | TYR | 171 | 17.634 | -0.469 | 76.407 | 1.00 | 41.17 | AAAA | C |
| ATOH | 1653 | CD2 | TYR | 171 | 16.065 | -2.429 | 75.194 | 1.00 | 43.62 | AAAA | C |
| ATOH | 1654 | CE2 | TYR | 171 | 16.734 | -2.675 | 76.366 | 1.00 | 44.44 | AAAA | C |
| ATOH | 1655 | CZ | TYR | 171 | 17.516 | -1.718 | 76.973 | 1.00 | 43.58 | AAAA | C |
| ATOH | 1656 | OH | TYR | 171 | 18.174 | -2.017 | 78.146 | 1.00 | 40.16 | AAAA | O |
| ATOH | 1658 | C | TYR | 171 | 17.058 | -1.938 | 71.832 | 1.00 | 51.41 | AAAA | C |
| ATOH | 1659 | O | TYR | 171 | 16.519 | -3.024 | 71.889 | 1.00 | 52.59 | AAAA | O |
| ATOH | 1660 | H | ASH | 172 | 18.331 | -1.752 | 71.493 | 1.00 | 53.70 | AAAA | H |
| ATOH | 1662 | CA | ASH | 172 | 19.203 | -2.898 | 71.193 | 1.00 | 52.36 | AAAA | C |
| ATOH | 1663 | CB | ASH | 172 | 19.085 | -3.278 | 69.709 | 1.00 | 55.43 | AAAA | C |
| ATOH | 1664 | CG | ASH | 172 | 18.939 | -4.766 | 69.498 | 1.00 | 61.75 | AAAA | C |
| ATOH | 1665 | OD1 | ASH | 172 | 19.233 | -5.646 | 70.304 | 1.00 | 61.61 | AAAA | O |
| ATOH | 1666 | HD2 | ASH | 172 | 18.449 | -5.048 | 68.295 | 1.00 | 57.97 | AAAA | H |
| ATOH | 1669 | C | ASH | 172 | 20.665 | -2.712 | 71.560 | 1.00 | 43.81 | AAAA | C |
| ATOH | 1670 | O | ASH | 172 | 21.163 | -1.760 | 72.213 | 1.00 | 39.38 | AAAA | O |
| ATOH | 1671 | H | TYR | 173 | 21.373 | -3.796 | 71.393 | 1.00 | 43.20 | AAAA | N |
| ATOH | 1673 | CA | TYR | 173 | 22.794 | -3.929 | 71.698 | 1.00 | 44.76 | AAAA | C |
| ATOH | 1674 | CB | TYR | 173 | 23.223 | -5.374 | 71.514 | 1.00 | 41.66 | AAAA | C |
| ATOH | 1675 | CG | TYR | 173 | 22.759 | -6.274 | 72.630 | 1.00 | 45.18 | AAAA | C |
| ATOH | 1676 | CD1 | TYR | 173 | 21.931 | -7.316 | 72.237 | 1.00 | 46.48 | AAAA | C |
| ATOH | 1677 | CE1 | TYR | 173 | 21.438 | -8.191 | 73.193 | 1.00 | 51.36 | AAAA | C |
| ATOH | 1678 | CD2 | TYR | 173 | 23.081 | -6.132 | 73.978 | 1.00 | 44.86 | AAAA | C |
| ATOH | 1679 | CE2 | TYR | 173 | 22.583 | -7.016 | 74.916 | 1.00 | 46.92 | AAAA | C |
| ATOH | 1680 | CZ | TYR | 173 | 21.757 | -8.038 | 74.535 | 1.00 | 50.33 | AAAA | C |
| ATOH | 1681 | OH | TYR | 173 | 21.171 | -9.006 | 75.328 | 1.00 | 50.64 | AAAA | O |
| ATOH | 1683 | C | TYR | 173 | 23.673 | -3.099 | 70.762 | 1.00 | 46.94 | AAAA | C |
| ATOH | 1684 | O | TYR | 173 | 23.389 | -2.983 | 69.567 | 1.00 | 49.76 | AAAA | O |
| ATOH | 1685 | H | ARG | 174 | 24.579 | -2.318 | 71.366 | 1.00 | 47.79 | AAAA | H |
| ATOH | 1687 | CA | ARG | 174 | 25.517 | -1.496 | 70.577 | 1.00 | 49.13 | AAAA | C |
| ATOH | 1688 | CB | ARG | 174 | 25.537 | -0.132 | 71.233 | 1.00 | 44.32 | AAAA | C |
| ATOH | 1689 | CG | ARG | 174 | 24.210 | 0.623 | 71.234 | 1.00 | 48.14 | AAAA | C |
| ATOH | 1690 | CD | ARG | 174 | 23.372 | 0.344 | 70.003 | 1.00 | 51.47 | AAAA | C |
| ATOH | 1691 | HE | ARG | 174 | 21.974 | 0.760 | 70.039 | 1.00 | 48.35 | AAAA | H |
| ATOH | 1693 | CG | ARG | 174 | 21.144 | 0.570 | 69.017 | 1.00 | 48.23 | AAAA | C |
| ATOH | 1694 | NH1 | ARG | 174 | 21.477 | 0.022 | 67.864 | 1.00 | 38.95 | AAAA | H |
| ATOH | 1697 | NH2 | ARG | 174 | 19.909 | 1.022 | 69.197 | 1.00 | 54.65 | AAAA | H |
| ATOH | 1700 | C | ARG | 174 | 26.921 | -2.094 | 70.461 | 1.00 | 45.98 | AAAA | C |
| ATOH | 1701 | O | ARG | 174 | 27.548 | -2.557 | 71.406 | 1.00 | 44.97 | AAAA | O |
| ATOH | 1702 | H | CYS | 175 | 27.493 | -2.183 | 69.294 | 1.00 | 46.21 | AAAA | H |
| ATOH | 1704 | CA | CYS | 175 | 28.787 | -2.758 | 68.997 | 1.00 | 45.60 | AAAA | C |
| ATOH | 1705 | C | CYS | 175 | 29.407 | -2.395 | 67.665 | 1.00 | 46.23 | AAAA | C |
| ATOH | 1706 | O | CYS | 175 | 28.755 | -2.018 | 66.665 | 1.00 | 44.78 | AAAA | O |
| ATOH | 1707 | CB | CYS | 175 | 28.576 | -4.253 | 69.167 | 1.00 | 35.62 | AAAA | C |
| ATOH | 1708 | SG | CYS | 175 | 27.812 | -5.191 | 67.927 | 1.00 | 51.92 | AAAA | S |
| ATOH | 1709 | H | TRP | 176 | 30.764 | -2.517 | 67.583 | 1.00 | 48.16 | AAAA | H |
| ATOH | 1711 | CA | TRP | 176 | 31.430 | -2.091 | 65.325 | 1.00 | 42.48 | AAAA | C |
| ATOH | 1712 | CB | TRP | 176 | 32.769 | -1.409 | 66.564 | 1.00 | 36.38 | AAAA | C |
| ATOH | 1713 | CG | TRP | 176 | 32.689 | -0.069 | 67.203 | 1.00 | 25.56 | AAAA | C |
| ATOH | 1714 | CD2 | TRP | 176 | 32.588 | 1.186 | 66.480 | 1.00 | 23.71 | AAAA | C |
| ATOH | 1715 | CE2 | TRP | 176 | 32.558 | 2.217 | 67.422 | 1.00 | 32.40 | AAAA | C |
| ATOH | 1716 | CE3 | TRP | 176 | 32.535 | 1.520 | 65.141 | 1.00 | 24.31 | AAAA | C |
| ATOH | 1717 | CD1 | TRP | 176 | 32.730 | 0.257 | 68.525 | 1.00 | 28.37 | AAAA | C |
| ATOH | 1718 | HE1 | TRP | 176 | 32.636 | 1.636 | 68.678 | 1.00 | 37.21 | AAAA | H |
| ATOH | 1720 | CG2 | TRP | 176 | 32.441 | 3.565 | 67.088 | 1.00 | 28.51 | AAAA | C |
| ATOH | 1721 | CG3 | TRP | 176 | 32.447 | 2.822 | 64.789 | 1.00 | 22.23 | AAAA | C |
| ATOH | 1722 | CH2 | TRP | 176 | 32.406 | 3.817 | 65.745 | 1.00 | 29.51 | AAAA | C |
| ATOH | 1723 | C | TRP | 176 | 31.631 | -3.268 | 65.408 | 1.00 | 39.30 | AAAA | C |
| ATOH | 1724 | O | TRP | 176 | 31.703 | -3.121 | 64.199 | 1.00 | 39.15 | AAAA | O |
| ATOH | 1725 | H | THR | 177 | 31.682 | -4.460 | 66.005 | 1.00 | 41.33 | AAAA | H |
| ATOH | 1727 | CA | THR | 177 | 31.964 | -5.644 | 65.161 | 1.00 | 49.28 | AAAA | C |
| ATOH | 1728 | CB | THR | 177 | 33.480 | -6.062 | 65.162 | 1.00 | 43.66 | AAAA | C |
| ATOH | 1729 | CG1 | THR | 177 | 34.309 | -5.025 | 64.613 | 1.00 | 47.85 | AAAA | O |
| ATOH | 1731 | CG2 | THR | 177 | 33.676 | -7.271 | 64.283 | 1.00 | 58.51 | AAAA | C |
| ATOH | 1732 | C | THR | 177 | 31.290 | -6.814 | 65.858 | 1.00 | 48.76 | AAAA | C |
| ATOH | 1733 | O | THR | 177 | 30.982 | -6.539 | 67.001 | 1.00 | 51.53 | AAAA | O |
| ATOH | 1734 | H | THR | 178 | 31.269 | -8.000 | 65.331 | 1.00 | 51.96 | AAAA | H |
| ATOH | 1736 | CA | THR | 178 | 30.924 | -9.236 | 65.946 | 1.00 | 58.95 | AAAA | C |
| ATOH | 1737 | CB | THR | 178 | 31.253 | -10.500 | 65.082 | 1.00 | 66.55 | AAAA | C |
| ATOH | 1738 | OG1 | THR | 178 | 31.505 | -10.066 | 63.734 | 1.00 | 75.70 | AAAA | O |
| ATOH | 1740 | CG2 | THR | 178 | 30.104 | -11.499 | 65.148 | 1.00 | 74.23 | AAAA | C |
| ATOH | 1741 | C | THR | 178 | 31.714 | -9.539 | 67.213 | 1.00 | 60.25 | AAAA | C |
| ATOH | 1742 | O | THR | 178 | 31.204 | -10.202 | 68.135 | 1.00 | 66.05 | AAAA | O |
| ATOH | 1743 | H | ASN | 179 | 32.977 | -9.130 | 67.253 | 1.00 | 57.56 | AAAA | H |
| ATOH | 1745 | CA | ASN | 179 | 33.793 | -9.392 | 68.443 | 1.00 | 53.39 | AAAA | C |
| ATOH | 1746 | CB | ASN | 179 | 35.130 | -10.024 | 68.068 | 1.00 | 48.46 | AAAA | C |
| ATOH | 1747 | CG | ASN | 179 | 34.897 | -11.218 | 67.126 | 1.00 | 56.25 | AAAA | C |
| ATOH | 1748 | OD1 | ASN | 179 | 34.412 | -12.294 | 67.553 | 1.00 | 51.38 | AAAA | O |
| ATOH | 1749 | HD2 | ASN | 179 | 35.229 | -11.063 | 65.863 | 1.00 | 48.10 | AAAA | H |
| ATOH | 1752 | C | ASH | 179 | 34.096 | -8.190 | 69.285 | 1.00 | 50.78 | AAAA | C |
| ATOH | 1753 | O | ASH | 179 | 34.556 | -8.377 | 70.426 | 1.00 | 57.97 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 1754 | H | ARG | 180 | 33.626 | -7.022 | 68.913 | 1.00 | 47.06 | AAAA | H |
| ATOM | 1755 | CA | ARG | 180 | 33.808 | -5.820 | 69.691 | 1.00 | 48.25 | AAAA | C |
| ATOM | 1757 | CB | ARG | 180 | 34.925 | -4.962 | 69.074 | 1.00 | 49.72 | AAAA | C |
| ATOM | 1758 | CG | ARG | 180 | 36.324 | -5.501 | 69.285 | 1.00 | 60.92 | AAAA | C |
| ATOM | 1759 | CD | ARG | 180 | 37.288 | -4.948 | 68.279 | 1.00 | 70.83 | AAAA | C |
| ATOM | 1760 | HE | ARG | 180 | 38.569 | -5.605 | 68.203 | 1.00 | 76.18 | AAAA | N |
| ATOM | 1762 | CE | ARG | 180 | 39.298 | -5.895 | 69.276 | 1.00 | 76.59 | AAAA | C |
| ATOM | 1763 | HH1 | ARG | 180 | 38.877 | -5.608 | 70.498 | 1.00 | 80.82 | AAAA | N |
| ATOM | 1766 | HH2 | ARG | 180 | 40.474 | -6.478 | 69.180 | 1.00 | 79.33 | AAAA | N |
| ATOM | 1769 | C | ARG | 180 | 32.530 | -4.977 | 69.821 | 1.00 | 48.10 | AAAA | C |
| ATOM | 1770 | O | ARG | 180 | 31.862 | -4.476 | 68.905 | 1.00 | 46.99 | AAAA | O |
| ATOM | 1771 | H | CYS | 181 | 32.230 | -4.728 | 71.063 | 1.00 | 44.80 | AAAA | H |
| ATOM | 1773 | CA | CYS | 181 | 31.199 | -3.924 | 71.619 | 1.00 | 45.20 | AAAA | C |
| ATOM | 1774 | C | CYS | 181 | 31.646 | -2.463 | 71.692 | 1.00 | 44.50 | AAAA | C |
| ATOM | 1775 | O | CYS | 181 | 32.835 | -2.227 | 71.724 | 1.00 | 47.09 | AAAA | O |
| ATOM | 1776 | CB | CYS | 181 | 30.940 | -4.282 | 73.110 | 1.00 | 43.88 | AAAA | C |
| ATOM | 1777 | SG | CYS | 181 | 30.363 | -5.944 | 73.346 | 1.00 | 56.08 | AAAA | S |
| ATOM | 1778 | H | GLN | 182 | 30.659 | -1.600 | 71.690 | 1.00 | 39.30 | AAAA | H |
| ATOM | 1780 | CA | GLN | 182 | 30.948 | -0.177 | 71.690 | 1.00 | 43.43 | AAAA | C |
| ATOM | 1781 | CB | GLN | 182 | 29.749 | 0.619 | 71.196 | 1.00 | 23.99 | AAAA | C |
| ATOM | 1782 | CG | GLN | 182 | 29.809 | 2.085 | 71.435 | 1.00 | 28.57 | AAAA | C |
| ATOM | 1783 | CD | GLN | 182 | 28.757 | 2.867 | 70.733 | 1.00 | 29.35 | AAAA | C |
| ATOM | 1784 | OE1 | GLN | 182 | 27.898 | 2.304 | 70.033 | 1.00 | 38.55 | AAAA | O |
| ATOM | 1785 | HE2 | GLN | 182 | 28.857 | 4.164 | 70.912 | 1.00 | 28.14 | AAAA | H |
| ATOM | 1788 | C | GLN | 182 | 31.218 | 0.089 | 73.162 | 1.00 | 46.07 | AAAA | C |
| ATOM | 1789 | O | GLN | 182 | 30.458 | -0.327 | 74.041 | 1.00 | 47.01 | AAAA | O |
| ATOM | 1790 | H | LYS | 183 | 32.213 | 0.866 | 73.524 | 1.00 | 46.98 | AAAA | H |
| ATOM | 1792 | CA | LYS | 183 | 32.479 | 1.064 | 74.934 | 1.00 | 45.26 | AAAA | C |
| ATOM | 1793 | CB | LYS | 183 | 33.966 | 1.275 | 75.185 | 1.00 | 48.68 | AAAA | C |
| ATOM | 1794 | CG | LYS | 183 | 34.865 | 0.267 | 74.482 | 1.00 | 47.95 | AAAA | C |
| ATOM | 1795 | CD | LYS | 183 | 36.337 | 0.734 | 74.523 | 1.00 | 48.06 | AAAA | C |
| ATOM | 1796 | CE | LYS | 183 | 37.178 | -0.208 | 73.684 | 1.00 | 46.78 | AAAA | C |
| ATOM | 1797 | HE | LYS | 183 | 38.499 | -0.654 | 74.158 | 1.00 | 44.00 | AAAA | H |
| ATOM | 1801 | C | LYS | 183 | 31.659 | 2.205 | 75.477 | 1.00 | 48.13 | AAAA | C |
| ATOM | 1802 | O | LYS | 183 | 31.679 | 3.305 | 74.946 | 1.00 | 48.84 | AAAA | O |
| ATOM | 1803 | H | NET | 184 | 31.165 | 2.014 | 76.699 | 1.00 | 52.59 | AAAA | H |
| ATOM | 1805 | CA | NET | 184 | 30.388 | 3.041 | 77.413 | 1.00 | 53.22 | AAAA | C |
| ATOM | 1806 | CB | NET | 184 | 28.927 | 2.613 | 77.537 | 1.00 | 54.27 | AAAA | C |
| ATOM | 1807 | CG | NET | 184 | 27.855 | 2.955 | 76.536 | 1.00 | 56.16 | AAAA | C |
| ATOM | 1818 | SD | NET | 184 | 26.911 | 1.601 | 75.912 | 1.00 | 57.56 | AAAA | S |
| ATOM | 1809 | CE | NET | 184 | 26.738 | 1.855 | 74.171 | 1.00 | 46.57 | AAAA | C |
| ATOM | 1810 | C | NET | 184 | 31.051 | 3.200 | 78.770 | 1.00 | 50.55 | AAAA | C |
| ATOM | 1811 | O | NET | 184 | 31.770 | 2.292 | 79.116 | 1.00 | 48.82 | AAAA | O |
| ATOM | 1812 | H | CYS | 185 | 30.796 | 4.195 | 79.565 | 1.00 | 53.97 | AAAA | H |
| ATOM | 1814 | CA | CYS | 185 | 31.342 | 4.365 | 80.892 | 1.00 | 58.63 | AAAA | C |
| ATOM | 1815 | C | CYS | 185 | 30.297 | 4.320 | 81.989 | 1.00 | 65.16 | AAAA | C |
| ATOM | 1816 | O | CYS | 185 | 29.133 | 4.649 | 81.761 | 1.00 | 65.87 | AAAA | O |
| ATOM | 1817 | CB | CYS | 185 | 31.965 | 5.772 | 81.000 | 1.00 | 60.37 | AAAA | C |
| ATOM | 1818 | SG | CYS | 185 | 33.623 | 5.771 | 80.312 | 1.00 | 60.09 | AAAA | S |
| ATOM | 1819 | H | PRO | 186 | 30.688 | 3.978 | 83.206 | 1.00 | 69.41 | AAAA | H |
| ATOM | 1820 | CD | PRO | 186 | 32.066 | 3.777 | 83.702 | 1.00 | 71.11 | AAAA | C |
| ATOM | 1821 | CA | PRO | 186 | 29.717 | 3.933 | 84.304 | 1.00 | 69.11 | AAAA | C |
| ATOM | 1822 | CB | PRO | 186 | 30.523 | 3.487 | 85.503 | 1.00 | 68.03 | AAAA | C |
| ATOM | 1823 | CG | PRO | 186 | 31.910 | 3.920 | 85.198 | 1.00 | 71.02 | AAAA | C |
| ATOM | 1824 | C | PRO | 186 | 29.120 | 5.320 | 84.431 | 1.00 | 69.47 | AAAA | C |
| ATOM | 1825 | O | PRO | 186 | 29.820 | 6.345 | 84.507 | 1.00 | 65.93 | AAAA | O |
| ATOM | 1826 | H | SER | 187 | 27.801 | 5.367 | 84.546 | 1.00 | 68.78 | AAAA | N |
| ATOM | 1828 | CA | SER | 187 | 27.050 | 6.592 | 84.750 | 1.00 | 69.29 | AAAA | C |
| ATOM | 1829 | CB | SER | 187 | 25.594 | 6.287 | 85.129 | 1.00 | 78.29 | AAAA | C |
| ATOM | 1830 | CG | SER | 187 | 25.474 | 4.935 | 85.566 | 1.00 | 91.78 | AAAA | O |
| ATOM | 1832 | C | SER | 187 | 27.630 | 7.476 | 85.836 | 1.00 | 67.19 | AAAA | C |
| ATOM | 1833 | O | SER | 187 | 27.606 | 8.708 | 85.803 | 1.00 | 63.98 | AAAA | O |
| ATOM | 1834 | N | THR | 188 | 28.108 | 6.853 | 86.908 | 1.00 | 68.20 | AAAA | N |
| ATOM | 1836 | CA | THR | 188 | 28.870 | 7.507 | 87.963 | 1.00 | 68.39 | AAAA | C |
| ATOM | 1837 | CB | THR | 188 | 29.805 | 6.459 | 88.618 | 1.00 | 73.84 | AAAA | C |
| ATOM | 1838 | CG1 | THR | 188 | 28.943 | 5.365 | 89.016 | 1.00 | 89.33 | AAAA | O |
| ATOM | 1840 | CG2 | THR | 188 | 30.605 | 7.048 | 89.759 | 1.00 | 73.71 | AAAA | C |
| ATOM | 1841 | C | THR | 188 | 29.802 | 8.583 | 87.429 | 1.00 | 67.52 | AAAA | C |
| ATOM | 1842 | O | THR | 188 | 29.843 | 9.739 | 87.834 | 1.00 | 68.30 | AAAA | O |
| ATOM | 1843 | N | CYS | 189 | 30.643 | 8.247 | 86.446 | 1.00 | 63.89 | AAAA | N |
| ATOM | 1845 | CA | CYS | 189 | 31.583 | 9.116 | 85.817 | 1.00 | 57.29 | AAAA | C |
| ATOM | 1846 | C | CYS | 189 | 30.951 | 10.331 | 85.195 | 1.00 | 57.70 | AAAA | C |
| ATOM | 1847 | O | CYS | 189 | 31.648 | 11.327 | 85.017 | 1.00 | 57.56 | AAAA | O |
| ATOM | 1848 | CB | CYS | 189 | 32.416 | 9.372 | 84.769 | 1.00 | 58.67 | AAAA | C |
| ATOM | 1849 | SG | CYS | 189 | 33.347 | 7.001 | 85.535 | 1.00 | 53.46 | AAAA | S |
| ATOM | 1850 | N | GLY | 190 | 29.689 | 10.322 | 84.806 | 1.00 | 56.91 | AAAA | N |
| ATOM | 1852 | CA | GLY | 190 | 29.038 | 11.521 | 84.323 | 1.00 | 57.28 | AAAA | C |
| ATOM | 1853 | C | GLY | 190 | 29.444 | 11.834 | 82.886 | 1.00 | 59.62 | AAAA | C |
| ATOM | 1854 | O | GLY | 190 | 29.609 | 10.932 | 82.082 | 1.00 | 57.91 | AAAA | O |
| ATOM | 1855 | H | LYS | 191 | 29.842 | 13.052 | 82.624 | 1.00 | 62.78 | AAAA | H |
| ATOM | 1857 | CA | LYS | 191 | 30.359 | 13.520 | 81.364 | 1.00 | 67.72 | AAAA | C |
| ATOM | 1858 | CB | LYS | 191 | 30.058 | 15.035 | 81.214 | 1.00 | 72.76 | AAAA | C |
| ATOM | 1859 | CG | LYS | 191 | 28.568 | 15.288 | 81.002 | 1.00 | 84.69 | AAAA | C |
| ATOM | 1860 | CD | LYS | 191 | 28.207 | 16.733 | 80.723 | 1.00 | 90.15 | AAAA | C |
| ATOM | 1861 | CE | LYS | 191 | 26.713 | 16.806 | 80.471 | 1.00 | 91.83 | AAAA | C |

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|------|------|------|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 1860 | HC | LYS | 191 | 26.368 | 16.182 | 79.152 | 1.00 | 97.62 | AAAA | H |
| ATOH | 1866 | C | LYS | 191 | 31.868 | 13.299 | 81.270 | 1.00 | 70.13 | AAAA | C |
| ATOH | 1867 | O | LYS | 191 | 32.486 | 13.935 | 80.415 | 1.00 | 71.76 | AAAA | O |
| ATOH | 1868 | H | ARG | 192 | 32.488 | 12.441 | 82.079 | 1.00 | 66.29 | AAAA | H |
| ATOH | 1870 | CA | ARG | 192 | 33.885 | 12.171 | 82.044 | 1.00 | 59.95 | AAAA | C |
| ATOH | 1871 | CB | ARG | 192 | 34.505 | 12.070 | 83.432 | 1.00 | 66.58 | AAAA | C |
| ATOH | 1872 | CG | ARG | 192 | 34.670 | 13.400 | 84.131 | 1.00 | 71.59 | AAAA | C |
| ATOH | 1873 | CD | ARG | 192 | 34.386 | 13.330 | 85.625 | 1.00 | 73.91 | AAAA | C |
| ATOH | 1874 | HE | ARG | 192 | 35.622 | 13.280 | 86.377 | 1.00 | 85.74 | AAAA | H |
| ATOH | 1876 | CZ | ARG | 192 | 35.968 | 12.407 | 87.330 | 1.00 | 90.67 | AAAA | C |
| ATOH | 1877 | IHH1 | ARG | 192 | 35.026 | 11.486 | 87.600 | 1.00 | 88.49 | AAAA | H |
| ATOH | 1880 | IHH2 | ARG | 192 | 37.162 | 12.463 | 87.950 | 1.00 | 72.95 | AAAA | H |
| ATOH | 1883 | C | ARG | 192 | 34.221 | 10.851 | 81.337 | 1.00 | 58.83 | AAAA | C |
| ATOH | 1884 | O | ARG | 192 | 33.336 | 10.007 | 81.176 | 1.00 | 55.13 | AAAA | O |
| ATOH | 1885 | H | ALA | 193 | 35.521 | 10.795 | 80.968 | 1.00 | 50.19 | AAAA | H |
| ATOH | 1887 | CA | ALA | 193 | 35.962 | 9.557 | 80.355 | 1.00 | 46.24 | AAAA | C |
| ATOH | 1888 | CB | ALA | 193 | 37.167 | 9.921 | 79.541 | 1.00 | 45.15 | AAAA | C |
| ATOH | 1889 | C | ALA | 193 | 36.221 | 8.525 | 81.451 | 1.00 | 48.97 | AAAA | C |
| ATOH | 1890 | O | ALA | 193 | 36.220 | 8.908 | 82.616 | 1.00 | 44.80 | AAAA | O |
| ATOH | 1891 | H | CYS | 194 | 36.544 | 7.304 | 81.065 | 1.00 | 50.30 | AAAA | H |
| ATOH | 1893 | CA | CYS | 194 | 36.836 | 6.302 | 82.043 | 1.00 | 57.50 | AAAA | C |
| ATOH | 1894 | C | CYS | 194 | 37.834 | 5.304 | 81.448 | 1.00 | 61.25 | AAAA | C |
| ATOH | 1895 | O | CYS | 194 | 37.952 | 5.291 | 80.216 | 1.00 | 61.52 | AAAA | O |
| ATOH | 1896 | CB | CYS | 194 | 35.510 | 5.741 | 82.504 | 1.00 | 57.96 | AAAA | C |
| ATOH | 1897 | SG | CYS | 194 | 34.785 | 4.524 | 81.402 | 1.00 | 54.49 | AAAA | S |
| ATOH | 1898 | H | THR | 195 | 38.422 | 4.499 | 82.311 | 1.00 | 58.51 | AAAA | H |
| ATOH | 1900 | CA | THR | 195 | 39.462 | 3.584 | 81.913 | 1.00 | 57.42 | AAAA | C |
| ATOH | 1901 | CB | THR | 195 | 40.237 | 3.142 | 83.188 | 1.00 | 65.73 | AAAA | C |
| ATOH | 1902 | CG1 | THR | 195 | 40.288 | 4.248 | 84.091 | 1.00 | 70.15 | AAAA | O |
| ATOH | 1904 | CG2 | THR | 195 | 41.684 | 2.864 | 82.745 | 1.00 | 77.91 | AAAA | C |
| ATOH | 1905 | C | THR | 195 | 38.857 | 2.404 | 81.226 | 1.00 | 54.59 | AAAA | C |
| ATOH | 1906 | O | THR | 195 | 37.633 | 2.315 | 81.318 | 1.00 | 58.75 | AAAA | O |
| ATOH | 1907 | H | GLU | 196 | 39.610 | 1.408 | 80.882 | 1.00 | 55.95 | AAAA | H |
| ATOH | 1909 | CA | GLU | 196 | 39.139 | 0.145 | 80.364 | 1.00 | 60.07 | AAAA | C |
| ATOH | 1910 | CB | GLU | 196 | 40.395 | -0.612 | 79.914 | 1.00 | 68.06 | AAAA | C |
| ATOH | 1911 | CG | GLU | 196 | 40.479 | -1.146 | 79.526 | 1.00 | 73.96 | AAAA | C |
| ATOH | 1912 | CD | GLU | 196 | 39.235 | -0.983 | 77.670 | 1.00 | 83.08 | AAAA | C |
| ATOH | 1913 | CE1 | GLU | 196 | 38.356 | -1.884 | 77.697 | 1.00 | 81.19 | AAAA | O |
| ATOH | 1914 | CE2 | GLU | 196 | 39.060 | 0.041 | 76.939 | 1.00 | 82.10 | AAAA | O |
| ATOH | 1915 | C | GLU | 196 | 38.382 | -0.579 | 81.467 | 1.00 | 63.91 | AAAA | C |
| ATOH | 1916 | O | GLU | 196 | 37.690 | -1.537 | 81.159 | 1.00 | 63.51 | AAAA | O |
| ATOH | 1917 | H | ASN | 197 | 39.666 | -0.312 | 82.739 | 1.00 | 67.40 | AAAA | H |
| ATOH | 1918 | CA | ASN | 197 | 38.025 | -0.947 | 83.886 | 1.00 | 69.21 | AAAA | C |
| ATOH | 1920 | CB | ASN | 197 | 39.021 | -1.394 | 84.966 | 1.00 | 68.49 | AAAA | C |
| ATOH | 1921 | CG | ASN | 197 | 39.722 | -2.692 | 84.672 | 0.01 | 69.09 | AAAA | C |
| ATOH | 1922 | CD1 | ASN | 197 | 40.364 | -3.273 | 85.551 | 0.01 | 69.04 | AAAA | O |
| ATOH | 1923 | HD2 | ASN | 197 | 39.622 | -3.193 | 93.443 | 0.01 | 68.97 | AAAA | H |
| ATOH | 1926 | C | ASN | 197 | 37.033 | 0.043 | 84.486 | 1.00 | 69.01 | AAAA | C |
| ATOH | 1927 | O | ASN | 197 | 36.945 | 0.281 | 85.664 | 1.00 | 68.24 | AAAA | O |
| ATOH | 1928 | H | ASN | 198 | 36.384 | 0.795 | 83.607 | 1.00 | 69.91 | AAAA | H |
| ATOH | 1930 | CA | ASN | 198 | 35.356 | 1.734 | 84.049 | 1.00 | 68.49 | AAAA | C |
| ATOH | 1931 | CB | ASN | 198 | 34.120 | 0.880 | 94.373 | 1.00 | 60.12 | AAAA | C |
| ATOH | 1932 | CG | ASN | 198 | 33.806 | 0.095 | 83.102 | 1.00 | 69.29 | AAAA | C |
| ATOH | 1933 | OD1 | ASN | 198 | 33.475 | 0.654 | 82.054 | 1.00 | 73.20 | AAAA | O |
| ATOH | 1934 | HD2 | ASN | 198 | 33.980 | -1.206 | 83.268 | 1.00 | 65.34 | AAAA | H |
| ATOH | 1937 | C | ASN | 198 | 35.784 | 2.563 | 85.228 | 1.00 | 64.01 | AAAA | C |
| ATOH | 1938 | O | ASN | 198 | 34.992 | 2.827 | 86.117 | 1.00 | 64.20 | AAAA | O |
| ATOH | 1939 | N | GLU | 199 | 36.955 | 3.164 | 85.157 | 1.00 | 64.75 | AAAA | N |
| ATOH | 1941 | CA | GLU | 199 | 37.342 | 4.054 | 86.255 | 1.00 | 64.64 | AAAA | C |
| ATOH | 1942 | CB | GLU | 199 | 38.702 | 3.624 | 86.744 | 1.00 | 66.11 | AAAA | C |
| ATOH | 1943 | CG | GLU | 199 | 38.846 | 3.717 | 88.233 | 1.00 | 77.15 | AAAA | C |
| ATOH | 1944 | CD | GLU | 199 | 39.579 | 2.532 | 88.832 | 1.00 | 80.24 | AAAA | C |
| ATOH | 1945 | OE1 | GLU | 199 | 39.385 | 2.406 | 90.066 | 1.00 | 81.65 | AAAA | O |
| ATOH | 1946 | OE2 | GLU | 199 | 40.282 | 1.821 | 88.079 | 1.00 | 77.94 | AAAA | O |
| ATOH | 1947 | C | GLU | 199 | 37.314 | 5.463 | 85.690 | 1.00 | 62.92 | AAAA | C |
| ATOH | 1948 | O | GLU | 199 | 37.922 | 5.676 | 84.632 | 1.00 | 63.62 | AAAA | O |
| ATOH | 1949 | H | CYS | 200 | 36.605 | 6.393 | 86.313 | 1.00 | 56.16 | AAAA | H |
| ATOH | 1951 | CA | CYS | 200 | 36.600 | 7.721 | 95.740 | 1.00 | 55.11 | AAAA | C |
| ATOH | 1952 | C | CYS | 200 | 37.978 | 8.315 | 85.521 | 1.00 | 57.77 | AAAA | C |
| ATOH | 1953 | O | CYS | 200 | 38.884 | 8.058 | 86.300 | 1.00 | 63.79 | AAAA | O |
| ATOH | 1954 | CB | CYS | 200 | 35.824 | 8.664 | 86.648 | 1.00 | 62.70 | AAAA | C |
| ATOH | 1955 | SG | CYS | 200 | 34.196 | 8.100 | 87.098 | 1.00 | 55.85 | AAAA | S |
| ATOH | 1956 | H | CYS | 201 | 38.124 | 9.192 | 84.540 | 1.00 | 54.50 | AAAA | H |
| ATOH | 1958 | CA | CYS | 201 | 39.338 | 9.399 | 84.202 | 1.00 | 48.19 | AAAA | C |
| ATOH | 1959 | C | CYS | 201 | 39.236 | 11.287 | 84.786 | 1.00 | 42.34 | AAAA | C |
| ATOH | 1960 | O | CYS | 201 | 38.165 | 11.704 | 85.166 | 1.00 | 54.32 | AAAA | O |
| ATOH | 1961 | CB | CYS | 201 | 39.590 | 10.070 | 82.695 | 1.00 | 40.90 | AAAA | C |
| ATOH | 1962 | SG | CYS | 201 | 39.644 | 8.597 | 81.747 | 1.00 | 51.42 | AAAA | S |
| ATOH | 1963 | H | HIS | 202 | 40.254 | 12.075 | 84.675 | 1.00 | 39.12 | AAAA | H |
| ATOH | 1965 | CA | HIS | 202 | 40.290 | 13.461 | 85.128 | 1.00 | 41.55 | AAAA | C |
| ATOH | 1966 | C | HIS | 202 | 39.284 | 14.184 | 84.289 | 1.00 | 46.59 | AAAA | C |
| ATOH | 1967 | O | HIS | 202 | 39.176 | 13.851 | 83.103 | 1.00 | 51.64 | AAAA | O |
| ATOH | 1968 | CB | HIS | 202 | 41.712 | 13.952 | 84.810 | 1.00 | 45.20 | AAAA | C |
| ATOH | 1969 | CG | HIS | 202 | 41.996 | 15.330 | 85.267 | 1.00 | 38.71 | AAAA | C |
| ATOH | 1970 | HD1 | HIS | 202 | 41.501 | 16.404 | 84.550 | 1.00 | 51.32 | AAAA | H |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 1971 | OE1 | HIS | 202 | 41.987 | 17.529 | 85.178 | 1.00 | 47.60 | AAAA | C |
| ATOM | 1972 | OD2 | HIS | 202 | 42.665 | 15.813 | 86.340 | 1.00 | 39.59 | AAAA | C |
| ATOM | 1973 | NE2 | HIS | 202 | 42.563 | 17.207 | 86.258 | 1.00 | 43.48 | AAAA | N |
| ATOM | 1975 | H | PRO | 203 | 38.738 | 15.293 | 84.711 | 1.00 | 47.74 | AAAA | N |
| ATOM | 1976 | CD | PRO | 203 | 38.758 | 15.840 | 86.082 | 1.00 | 46.97 | AAAA | C |
| ATOM | 1977 | CA | PRO | 203 | 37.780 | 15.987 | 83.879 | 1.00 | 46.44 | AAAA | C |
| ATOM | 1978 | CB | PRO | 203 | 37.248 | 17.107 | 84.742 | 1.00 | 39.47 | AAAA | C |
| ATOM | 1979 | CG | PRO | 203 | 38.131 | 17.210 | 85.910 | 1.00 | 43.37 | AAAA | C |
| ATOM | 1980 | C | PRO | 203 | 38.440 | 16.519 | 82.607 | 1.00 | 53.27 | AAAA | C |
| ATOM | 1981 | O | PRO | 203 | 37.698 | 17.045 | 81.731 | 1.00 | 53.16 | AAAA | O |
| ATOM | 1982 | H | GLU | 204 | 39.792 | 16.535 | 82.561 | 1.00 | 50.34 | AAAA | N |
| ATOM | 1984 | CA | GLU | 204 | 40.439 | 17.139 | 81.381 | 1.00 | 50.52 | AAAA | C |
| ATOM | 1985 | CB | GLU | 204 | 41.727 | 17.891 | 81.804 | 1.00 | 48.58 | AAAA | C |
| ATOM | 1986 | CG | GLU | 204 | 41.397 | 19.251 | 82.397 | 1.00 | 43.74 | AAAA | C |
| ATOM | 1987 | CD | GLU | 204 | 40.778 | 20.282 | 81.501 | 1.00 | 55.26 | AAAA | C |
| ATOM | 1988 | OE1 | GLU | 204 | 40.766 | 20.344 | 80.248 | 1.00 | 64.04 | AAAA | O |
| ATOM | 1989 | OE2 | GLU | 204 | 40.226 | 21.198 | 82.141 | 1.00 | 57.66 | AAAA | O |
| ATOM | 1990 | C | GLU | 204 | 40.718 | 16.084 | 80.319 | 1.00 | 45.71 | AAAA | C |
| ATOM | 1991 | O | GLU | 204 | 41.238 | 16.405 | 79.251 | 1.00 | 46.56 | AAAA | O |
| ATOM | 1992 | H | CYS | 205 | 40.612 | 14.830 | 80.735 | 1.00 | 42.05 | AAAA | H |
| ATOM | 1994 | CA | CYS | 205 | 40.997 | 13.764 | 79.838 | 1.00 | 45.81 | AAAA | C |
| ATOM | 1995 | C | CYS | 205 | 39.892 | 13.628 | 78.819 | 1.00 | 49.20 | AAAA | C |
| ATOM | 1996 | O | CYS | 205 | 38.746 | 13.920 | 79.133 | 1.00 | 50.34 | AAAA | O |
| ATOM | 1997 | CB | CYS | 205 | 41.288 | 12.491 | 80.572 | 1.00 | 51.55 | AAAA | C |
| ATOM | 1998 | SG | CYS | 205 | 42.923 | 12.246 | 81.251 | 1.00 | 52.89 | AAAA | S |
| ATOM | 1999 | H | LEU | 206 | 40.232 | 13.579 | 77.520 | 1.00 | 49.88 | AAAA | H |
| ATOM | 2001 | CA | LEU | 206 | 39.169 | 13.446 | 76.533 | 1.00 | 41.49 | AAAA | C |
| ATOM | 2002 | CB | LEU | 206 | 39.266 | 14.505 | 75.462 | 1.00 | 48.66 | AAAA | C |
| ATOM | 2003 | CG | LEU | 206 | 38.274 | 14.365 | 74.305 | 1.00 | 47.45 | AAAA | C |
| ATOM | 2004 | CD1 | LEU | 206 | 36.879 | 14.243 | 74.895 | 1.00 | 45.79 | AAAA | C |
| ATOM | 2005 | CD2 | LEU | 206 | 38.331 | 15.599 | 73.420 | 1.00 | 50.71 | AAAA | C |
| ATOM | 2006 | C | LEU | 206 | 39.310 | 12.109 | 75.912 | 1.00 | 38.44 | AAAA | C |
| ATOM | 2007 | O | LEU | 206 | 40.400 | 11.568 | 75.813 | 1.00 | 36.59 | AAAA | O |
| ATOM | 2008 | H | GLY | 207 | 38.264 | 11.359 | 75.681 | 1.00 | 42.41 | AAAA | H |
| ATOM | 2010 | CA | GLY | 207 | 38.403 | 10.098 | 74.979 | 1.00 | 40.57 | AAAA | C |
| ATOM | 2011 | C | GLY | 207 | 38.466 | 9.061 | 76.058 | 1.00 | 47.15 | AAAA | C |
| ATOM | 2012 | O | GLY | 207 | 37.668 | 9.102 | 76.057 | 1.00 | 45.04 | AAAA | O |
| ATOM | 2013 | H | SER | 208 | 39.622 | 9.079 | 76.760 | 1.00 | 50.36 | AAAA | H |
| ATOM | 2015 | CA | SER | 208 | 39.832 | 7.838 | 77.660 | 1.00 | 48.27 | AAAA | C |
| ATOM | 2016 | CB | SER | 208 | 39.909 | 6.631 | 76.787 | 1.00 | 35.77 | AAAA | C |
| ATOM | 2017 | CG | SER | 208 | 40.600 | 5.597 | 77.461 | 1.00 | 61.34 | AAAA | O |
| ATOM | 2019 | C | SER | 208 | 41.144 | 8.068 | 78.377 | 1.00 | 49.17 | AAAA | C |
| ATOM | 2020 | O | SER | 208 | 41.781 | 9.084 | 78.163 | 1.00 | 48.24 | AAAA | O |
| ATOM | 2021 | H | CYS | 209 | 41.599 | 7.123 | 79.199 | 1.00 | 52.04 | AAAA | H |
| ATOM | 2023 | CA | CYS | 209 | 42.924 | 7.307 | 79.964 | 1.00 | 55.98 | AAAA | C |
| ATOM | 2024 | C | CYS | 209 | 43.453 | 6.035 | 80.484 | 1.00 | 57.41 | AAAA | C |
| ATOM | 2025 | O | CYS | 209 | 42.962 | 4.963 | 80.423 | 1.00 | 58.33 | AAAA | O |
| ATOM | 2026 | CB | CYS | 209 | 42.629 | 9.058 | 81.146 | 1.00 | 52.51 | AAAA | C |
| ATOM | 2027 | SG | CYS | 209 | 41.380 | 7.602 | 82.261 | 1.00 | 58.22 | AAAA | S |
| ATOM | 2028 | H | SER | 210 | 44.734 | 6.145 | 80.893 | 1.00 | 59.37 | AAAA | N |
| ATOM | 2030 | CA | SER | 210 | 45.506 | 4.950 | 81.319 | 1.00 | 58.10 | AAAA | C |
| ATOM | 2031 | CB | SER | 210 | 47.022 | 5.093 | 81.105 | 1.00 | 55.07 | AAAA | C |
| ATOM | 2032 | CG | SER | 210 | 47.546 | 6.204 | 81.819 | 1.00 | 64.49 | AAAA | O |
| ATOM | 2034 | C | SER | 210 | 45.331 | 4.713 | 82.826 | 1.00 | 56.34 | AAAA | C |
| ATOM | 2035 | O | SER | 210 | 45.529 | 3.614 | 83.326 | 1.00 | 54.42 | AAAA | O |
| ATOM | 2036 | H | ALA | 211 | 45.105 | 5.806 | 83.548 | 1.00 | 52.79 | AAAA | N |
| ATOM | 2038 | CA | ALA | 211 | 44.980 | 5.684 | 85.004 | 1.00 | 56.60 | AAAA | C |
| ATOM | 2039 | CB | ALA | 211 | 46.333 | 5.926 | 85.649 | 1.00 | 63.41 | AAAA | C |
| ATOM | 2040 | C | ALA | 211 | 43.962 | 6.747 | 85.395 | 1.00 | 56.58 | AAAA | C |
| ATOM | 2041 | O | ALA | 211 | 43.957 | 7.792 | 84.711 | 1.00 | 50.78 | AAAA | O |
| ATOM | 2042 | H | PRO | 212 | 43.117 | 6.416 | 86.359 | 1.00 | 55.93 | AAAA | N |
| ATOM | 2043 | CD | PRO | 212 | 43.042 | 5.166 | 87.115 | 1.00 | 55.86 | AAAA | C |
| ATOM | 2044 | CA | PRO | 212 | 41.951 | 7.257 | 86.575 | 1.00 | 55.50 | AAAA | C |
| ATOM | 2045 | CB | PRO | 212 | 41.104 | 6.470 | 87.556 | 1.00 | 59.65 | AAAA | C |
| ATOM | 2046 | CG | PRO | 212 | 42.021 | 5.493 | 88.175 | 1.00 | 54.56 | AAAA | C |
| ATOM | 2047 | C | PRO | 212 | 42.409 | 8.535 | 87.177 | 1.00 | 53.64 | AAAA | C |
| ATOM | 2048 | O | PRO | 212 | 43.611 | 8.725 | 87.393 | 1.00 | 57.48 | AAAA | O |
| ATOM | 2049 | H | ALA | 213 | 41.537 | 9.492 | 87.347 | 1.00 | 53.87 | AAAA | N |
| ATOM | 2051 | CA | ALA | 213 | 41.912 | 10.710 | 88.057 | 1.00 | 59.41 | AAAA | C |
| ATOM | 2052 | CB | ALA | 213 | 41.783 | 10.255 | 89.541 | 1.00 | 66.40 | AAAA | C |
| ATOM | 2053 | C | ALA | 213 | 43.289 | 11.300 | 87.907 | 1.00 | 61.40 | AAAA | C |
| ATOM | 2054 | O | ALA | 213 | 43.728 | 12.202 | 88.652 | 1.00 | 60.03 | AAAA | O |
| ATOM | 2055 | H | ASH | 214 | 44.068 | 10.999 | 86.899 | 1.00 | 64.80 | AAAA | N |
| ATOM | 2057 | CA | ASH | 214 | 45.366 | 11.551 | 86.596 | 1.00 | 63.36 | AAAA | C |
| ATOM | 2063 | C | ASH | 214 | 45.300 | 12.294 | 85.251 | 1.00 | 61.56 | AAAA | C |
| ATOM | 2064 | O | ASH | 214 | 45.198 | 11.794 | 84.117 | 1.00 | 58.38 | AAAA | O |
| ATOM | 2058 | CB | ASH | 214 | 46.336 | 10.379 | 86.608 | 1.00 | 67.32 | AAAA | C |
| ATOM | 2059 | CG | ASH | 214 | 47.697 | 10.896 | 86.362 | 1.00 | 75.48 | AAAA | C |
| ATOM | 2060 | OD1 | ASH | 214 | 48.254 | 11.105 | 85.302 | 1.00 | 83.64 | AAAA | O |
| ATOM | 2061 | HD2 | ASH | 214 | 48.513 | 11.170 | 87.427 | 1.00 | 90.05 | AAAA | N |
| ATOM | 2065 | H | ASP | 215 | 45.666 | 13.565 | 85.305 | 1.00 | 59.78 | AAAA | H |
| ATOM | 2067 | CA | ASP | 215 | 45.618 | 14.432 | 84.143 | 1.00 | 56.47 | AAAA | C |
| ATOM | 2068 | CB | ASP | 215 | 45.430 | 15.926 | 84.446 | 1.00 | 40.19 | AAAA | C |
| ATOM | 2069 | CG | ASP | 215 | 46.671 | 16.543 | 84.986 | 1.00 | 56.36 | AAAA | C |
| ATOM | 2070 | OD1 | ASP | 215 | 46.590 | 17.699 | 85.473 | 1.00 | 56.17 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 2071 | OC | ASP | 215 | 47.766 | 15.926 | 84.941 | 1.00 | 60.51 | AAAA | O |
| ATOM | 2072 | O | ASP | 215 | 46.818 | 14.315 | 83.221 | 1.00 | 53.79 | AAAA | C |
| ATOM | 2073 | O | ASP | 215 | 46.998 | 15.148 | 82.322 | 1.00 | 53.58 | AAAA | O |
| ATOM | 2074 | H | THR | 216 | 47.719 | 13.425 | 83.511 | 1.00 | 50.87 | AAAA | H |
| ATOM | 2076 | CA | THR | 216 | 48.883 | 13.114 | 82.734 | 1.00 | 45.76 | AAAA | C |
| ATOM | 2077 | CB | THR | 216 | 50.201 | 13.176 | 83.529 | 1.00 | 53.46 | AAAA | C |
| ATOM | 2078 | CG1 | THR | 216 | 50.403 | 11.977 | 84.335 | 1.00 | 45.14 | AAAA | O |
| ATOM | 2080 | CG2 | THR | 216 | 50.436 | 14.314 | 84.518 | 1.00 | 41.38 | AAAA | C |
| ATOM | 2081 | O | THR | 216 | 48.681 | 11.712 | 82.158 | 1.00 | 48.34 | AAAA | C |
| ATOM | 2082 | O | THR | 216 | 49.596 | 11.282 | 81.444 | 1.00 | 47.49 | AAAA | O |
| ATOM | 2083 | H | ALA | 217 | 47.559 | 11.057 | 82.476 | 1.00 | 49.65 | AAAA | N |
| ATOM | 2085 | CA | ALA | 217 | 47.259 | 9.760 | 81.845 | 1.00 | 51.83 | AAAA | C |
| ATOM | 2086 | CB | ALA | 217 | 46.908 | 8.775 | 82.943 | 1.00 | 52.62 | AAAA | C |
| ATOM | 2087 | C | ALA | 217 | 46.207 | 9.747 | 80.709 | 1.00 | 50.60 | AAAA | C |
| ATOM | 2089 | O | ALA | 217 | 45.775 | 8.632 | 80.335 | 1.00 | 49.13 | AAAA | O |
| ATOM | 2089 | H | CYS | 218 | 45.744 | 10.905 | 80.226 | 1.00 | 43.56 | AAAA | H |
| ATOM | 2091 | CA | CYS | 218 | 44.802 | 11.030 | 79.157 | 1.00 | 48.09 | AAAA | C |
| ATOM | 2092 | C | CYS | 218 | 45.166 | 10.331 | 77.869 | 1.00 | 47.06 | AAAA | C |
| ATOM | 2093 | O | CYS | 218 | 46.300 | 9.967 | 77.642 | 1.00 | 55.57 | AAAA | O |
| ATOM | 2094 | CB | CYS | 218 | 44.536 | 12.501 | 78.775 | 1.00 | 51.54 | AAAA | C |
| ATOM | 2095 | SG | CYS | 218 | 44.256 | 13.494 | 80.302 | 1.00 | 56.98 | AAAA | S |
| ATOM | 2096 | H | VAL | 219 | 44.226 | 10.085 | 76.978 | 1.00 | 43.40 | AAAA | H |
| ATOM | 2098 | CA | VAL | 219 | 44.575 | 9.547 | 75.654 | 1.00 | 35.22 | AAAA | C |
| ATOM | 2099 | CB | VAL | 219 | 43.693 | 8.427 | 75.242 | 1.00 | 32.26 | AAAA | C |
| ATOM | 2100 | CG1 | VAL | 219 | 43.952 | 7.873 | 73.886 | 1.00 | 36.19 | AAAA | C |
| ATOM | 2101 | CG2 | VAL | 219 | 43.811 | 7.144 | 76.071 | 1.00 | 45.51 | AAAA | C |
| ATOM | 2102 | C | VAL | 219 | 44.453 | 10.750 | 74.735 | 1.00 | 32.06 | AAAA | C |
| ATOM | 2103 | O | VAL | 219 | 45.303 | 10.897 | 73.874 | 1.00 | 42.27 | AAAA | O |
| ATOM | 2104 | H | ALA | 220 | 43.728 | 11.759 | 75.187 | 1.00 | 24.24 | AAAA | H |
| ATOM | 2106 | CA | ALA | 220 | 43.630 | 12.985 | 74.385 | 1.00 | 27.99 | AAAA | C |
| ATOM | 2107 | CB | ALA | 220 | 42.536 | 12.919 | 73.331 | 1.00 | 28.42 | AAAA | C |
| ATOM | 2108 | C | ALA | 220 | 43.292 | 14.671 | 75.390 | 1.00 | 29.21 | AAAA | C |
| ATOM | 2109 | O | ALA | 220 | 42.846 | 13.604 | 76.455 | 1.00 | 37.88 | AAAA | O |
| ATOM | 2110 | H | CYS | 221 | 43.285 | 15.334 | 75.059 | 1.00 | 30.27 | AAAA | H |
| ATOM | 2112 | CA | CYS | 221 | 42.753 | 16.392 | 75.875 | 1.00 | 35.55 | AAAA | C |
| ATOM | 2113 | C | CYS | 221 | 41.460 | 17.055 | 75.452 | 1.00 | 47.06 | AAAA | C |
| ATOM | 2114 | O | CYS | 221 | 41.265 | 17.598 | 74.369 | 1.00 | 49.57 | AAAA | O |
| ATOM | 2115 | CB | CYS | 221 | 43.804 | 17.479 | 76.063 | 1.00 | 47.45 | AAAA | C |
| ATOM | 2116 | SG | CYS | 221 | 45.494 | 16.935 | 76.538 | 1.00 | 47.66 | AAAA | S |
| ATOM | 2117 | H | ARG | 222 | 40.503 | 17.133 | 76.396 | 1.00 | 51.47 | AAAA | N |
| ATOM | 2119 | CA | ARG | 222 | 39.281 | 17.906 | 76.339 | 1.00 | 51.86 | AAAA | C |
| ATOM | 2120 | CB | ARG | 222 | 38.647 | 19.674 | 77.712 | 1.00 | 54.53 | AAAA | C |
| ATOM | 2121 | CG | ARG | 222 | 37.314 | 19.697 | 77.854 | 1.00 | 45.56 | AAAA | C |
| ATOM | 2122 | CD | ARG | 222 | 36.538 | 19.338 | 79.087 | 1.00 | 54.45 | AAAA | C |
| ATOM | 2123 | NE | ARG | 222 | 36.272 | 16.947 | 79.269 | 1.00 | 65.53 | AAAA | H |
| ATOM | 2125 | CD | ARG | 222 | 35.534 | 16.080 | 78.617 | 1.00 | 67.60 | AAAA | C |
| ATOM | 2126 | HN1 | ARG | 222 | 34.925 | 16.599 | 77.533 | 1.00 | 70.26 | AAAA | H |
| ATOM | 2129 | HN2 | ARG | 222 | 35.342 | 14.780 | 78.901 | 1.00 | 54.11 | AAAA | H |
| ATOM | 2130 | C | ARG | 222 | 39.562 | 19.286 | 75.740 | 1.00 | 50.66 | AAAA | C |
| ATOM | 2133 | O | ARG | 222 | 39.737 | 19.845 | 75.009 | 1.00 | 58.34 | AAAA | O |
| ATOM | 2134 | H | HIS | 223 | 40.556 | 19.921 | 76.190 | 1.00 | 45.65 | AAAA | H |
| ATOM | 2136 | CA | HIS | 223 | 40.988 | 21.291 | 75.821 | 1.00 | 46.93 | AAAA | C |
| ATOM | 2137 | CB | HIS | 223 | 41.057 | 22.251 | 77.011 | 1.00 | 49.51 | AAAA | C |
| ATOM | 2139 | CG | HIS | 223 | 39.710 | 22.344 | 77.647 | 1.00 | 58.83 | AAAA | C |
| ATOM | 2139 | CD2 | HIS | 223 | 38.820 | 23.360 | 77.556 | 1.00 | 61.08 | AAAA | C |
| ATOM | 2140 | HN1 | HIS | 223 | 39.082 | 21.388 | 78.425 | 1.00 | 63.28 | AAAA | H |
| ATOM | 2142 | CE1 | HIS | 223 | 37.881 | 21.915 | 78.759 | 1.00 | 58.01 | AAAA | C |
| ATOM | 2143 | NE2 | HIS | 223 | 37.681 | 23.010 | 78.232 | 1.00 | 48.56 | AAAA | N |
| ATOM | 2145 | O | HIS | 223 | 42.363 | 21.260 | 75.122 | 1.00 | 50.79 | AAAA | C |
| ATOM | 2146 | O | HIS | 223 | 42.506 | 20.753 | 74.003 | 1.00 | 47.43 | AAAA | O |
| ATOM | 2147 | H | TYR | 224 | 43.359 | 21.847 | 75.769 | 1.00 | 49.20 | AAAA | H |
| ATOM | 2149 | CA | TYR | 224 | 44.712 | 21.992 | 75.259 | 1.00 | 48.17 | AAAA | C |
| ATOM | 2150 | CB | TYR | 224 | 45.144 | 23.430 | 75.426 | 1.00 | 44.07 | AAAA | C |
| ATOM | 2151 | CG | TYR | 224 | 44.318 | 24.234 | 74.417 | 1.00 | 51.77 | AAAA | C |
| ATOM | 2152 | CD1 | TYR | 224 | 43.193 | 24.869 | 74.904 | 1.00 | 48.94 | AAAA | C |
| ATOM | 2153 | CE1 | TYR | 224 | 42.401 | 25.633 | 74.089 | 1.00 | 48.41 | AAAA | C |
| ATOM | 2154 | CD2 | TYR | 224 | 44.623 | 24.358 | 73.065 | 1.00 | 54.82 | AAAA | C |
| ATOM | 2155 | CE2 | TYR | 224 | 43.847 | 25.131 | 72.233 | 1.00 | 56.09 | AAAA | C |
| ATOM | 2156 | CD | TYR | 224 | 42.739 | 25.745 | 72.766 | 1.00 | 54.23 | AAAA | C |
| ATOM | 2157 | OH | TYR | 224 | 41.915 | 26.522 | 72.017 | 1.00 | 61.70 | AAAA | O |
| ATOM | 2159 | O | TYR | 224 | 45.725 | 21.095 | 75.892 | 1.00 | 48.19 | AAAA | C |
| ATOM | 2160 | O | TYR | 224 | 45.776 | 20.913 | 77.111 | 1.00 | 55.75 | AAAA | O |
| ATOM | 2161 | H | TYR | 225 | 46.584 | 20.514 | 75.077 | 1.00 | 48.79 | AAAA | N |
| ATOM | 2163 | CA | TYR | 225 | 47.655 | 19.653 | 75.555 | 1.00 | 43.02 | AAAA | C |
| ATOM | 2164 | CB | TYR | 225 | 48.020 | 18.639 | 74.548 | 1.00 | 42.32 | AAAA | C |
| ATOM | 2165 | CG | TYR | 225 | 49.286 | 17.926 | 74.954 | 1.00 | 46.95 | AAAA | C |
| ATOM | 2166 | CD1 | TYR | 225 | 49.299 | 16.858 | 75.817 | 1.00 | 43.57 | AAAA | C |
| ATOM | 2167 | CE1 | TYR | 225 | 50.450 | 16.221 | 76.173 | 1.00 | 47.26 | AAAA | C |
| ATOM | 2168 | CD2 | TYR | 225 | 50.487 | 18.407 | 74.421 | 1.00 | 52.82 | AAAA | C |
| ATOM | 2169 | CE2 | TYR | 225 | 51.656 | 17.791 | 74.781 | 1.00 | 53.94 | AAAA | C |
| ATOM | 2170 | CD | TYR | 225 | 51.639 | 16.707 | 75.644 | 1.00 | 52.31 | AAAA | C |
| ATOM | 2171 | OH | TYR | 225 | 52.886 | 16.186 | 75.905 | 1.00 | 50.71 | AAAA | O |
| ATOM | 2173 | C | TYR | 225 | 48.872 | 20.507 | 75.793 | 1.00 | 47.13 | AAAA | C |
| ATOM | 2174 | O | TYR | 225 | 49.080 | 21.514 | 75.150 | 1.00 | 53.97 | AAAA | O |
| ATOM | 2175 | H | TYR | 226 | 49.634 | 20.253 | 76.821 | 1.00 | 56.84 | AAAA | H |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 2177 | CA | TYR | 226 | 50.814 | 21.001 | 77.172 | 1.00 | 56.23 | AAAA | C |
| ATOH | 2178 | TR | TYR | 226 | 50.455 | 22.343 | 77.785 | 1.00 | 59.51 | AAAA | C |
| ATOH | 2179 | CG | TYR | 226 | 51.741 | 23.126 | 77.941 | 1.00 | 65.45 | AAAA | C |
| ATOH | 2180 | CD1 | TYR | 226 | 52.121 | 23.557 | 79.197 | 1.00 | 69.12 | AAAA | C |
| ATOH | 2181 | CE1 | TYR | 226 | 53.289 | 24.275 | 79.400 | 1.00 | 70.77 | AAAA | C |
| ATOH | 2182 | CD2 | TYR | 226 | 52.580 | 23.409 | 76.864 | 1.00 | 69.38 | AAAA | C |
| ATOH | 2183 | CE2 | TYR | 226 | 53.758 | 24.118 | 77.020 | 1.00 | 70.94 | AAAA | C |
| ATOH | 2184 | CG | TYR | 226 | 54.099 | 24.549 | 78.301 | 1.00 | 72.96 | AAAA | C |
| ATOH | 2185 | OH | TYR | 226 | 55.267 | 25.254 | 78.435 | 1.00 | 70.84 | AAAA | O |
| ATOH | 2187 | C | TYR | 226 | 51.784 | 20.356 | 78.165 | 1.00 | 57.55 | AAAA | C |
| ATOH | 2188 | O | TYR | 226 | 51.492 | 20.133 | 79.350 | 1.00 | 56.90 | AAAA | O |
| ATOH | 2189 | H | ALA | 227 | 52.978 | 20.080 | 77.642 | 1.00 | 53.82 | AAAA | N |
| ATOH | 2191 | CA | ALA | 227 | 54.061 | 19.557 | 78.440 | 1.00 | 51.82 | AAAA | C |
| ATOH | 2192 | CB | ALA | 227 | 54.528 | 20.620 | 79.428 | 1.00 | 55.81 | AAAA | C |
| ATOH | 2193 | C | ALA | 227 | 53.600 | 18.309 | 79.170 | 1.00 | 53.56 | AAAA | C |
| ATOH | 2194 | O | ALA | 227 | 53.663 | 18.218 | 80.413 | 1.00 | 49.63 | AAAA | O |
| ATOH | 2195 | H | GLY | 228 | 53.076 | 17.360 | 78.393 | 1.00 | 50.68 | AAAA | N |
| ATOH | 2197 | CA | GLY | 228 | 52.585 | 16.135 | 79.028 | 1.00 | 49.02 | AAAA | C |
| ATOH | 2198 | C | GLY | 228 | 51.312 | 16.330 | 79.861 | 1.00 | 51.61 | AAAA | C |
| ATOH | 2199 | O | GLY | 228 | 51.028 | 15.538 | 80.776 | 1.00 | 51.10 | AAAA | O |
| ATOH | 2200 | H | VAL | 229 | 50.643 | 17.495 | 79.791 | 1.00 | 47.09 | AAAA | N |
| ATOH | 2202 | CA | VAL | 229 | 49.489 | 17.671 | 80.635 | 1.00 | 51.11 | AAAA | C |
| ATOH | 2203 | CB | VAL | 229 | 49.908 | 18.610 | 81.774 | 1.00 | 56.52 | AAAA | C |
| ATOH | 2204 | CG1 | VAL | 229 | 48.627 | 18.896 | 82.566 | 1.00 | 38.39 | AAAA | C |
| ATOH | 2205 | CG2 | VAL | 229 | 51.002 | 18.035 | 82.682 | 1.00 | 50.16 | AAAA | C |
| ATOH | 2206 | C | VAL | 229 | 48.255 | 18.173 | 79.873 | 1.00 | 51.37 | AAAA | C |
| ATOH | 2207 | O | VAL | 229 | 48.344 | 19.279 | 79.309 | 1.00 | 53.71 | AAAA | O |
| ATOH | 2208 | H | CYS | 230 | 47.100 | 17.518 | 80.036 | 1.00 | 42.21 | AAAA | N |
| ATOH | 2210 | CA | CYS | 230 | 45.881 | 18.117 | 79.471 | 1.00 | 40.32 | AAAA | C |
| ATOH | 2211 | C | CYS | 230 | 45.456 | 19.350 | 80.228 | 1.00 | 38.42 | AAAA | C |
| ATOH | 2212 | O | CYS | 230 | 44.964 | 19.248 | 81.321 | 1.00 | 41.62 | AAAA | O |
| ATOH | 2213 | CB | CYS | 230 | 44.746 | 17.132 | 79.370 | 1.00 | 31.54 | AAAA | C |
| ATOH | 2214 | SG | CYS | 230 | 45.149 | 15.753 | 78.266 | 1.00 | 43.61 | AAAA | S |
| ATOH | 2215 | H | VAL | 231 | 45.637 | 20.534 | 79.731 | 1.00 | 39.83 | AAAA | N |
| ATOH | 2217 | CA | VAL | 231 | 45.445 | 21.769 | 80.462 | 1.00 | 46.57 | AAAA | C |
| ATOH | 2218 | CB | VAL | 231 | 46.619 | 22.736 | 80.089 | 1.00 | 50.99 | AAAA | C |
| ATOH | 2219 | CG1 | VAL | 231 | 46.798 | 23.878 | 81.053 | 1.00 | 50.41 | AAAA | C |
| ATOH | 2220 | CG2 | VAL | 231 | 47.839 | 21.913 | 80.506 | 1.00 | 44.95 | AAAA | C |
| ATOH | 2221 | C | VAL | 231 | 44.111 | 22.321 | 80.057 | 1.00 | 52.59 | AAAA | C |
| ATOH | 2222 | O | VAL | 231 | 43.999 | 22.193 | 78.936 | 1.00 | 55.30 | AAAA | O |
| ATOH | 2223 | H | PRO | 232 | 43.482 | 23.105 | 80.913 | 1.00 | 54.28 | AAAA | N |
| ATOH | 2224 | CD | PRO | 232 | 43.930 | 23.385 | 82.320 | 1.00 | 54.25 | AAAA | C |
| ATOH | 2225 | CA | PRO | 232 | 42.153 | 23.626 | 80.575 | 1.00 | 54.39 | AAAA | C |
| ATOH | 2226 | CB | PRO | 232 | 41.537 | 23.877 | 81.928 | 1.00 | 53.73 | AAAA | C |
| ATOH | 2227 | CG | PRO | 232 | 42.683 | 24.287 | 82.765 | 1.00 | 55.60 | AAAA | C |
| ATOH | 2228 | C | PRO | 232 | 42.361 | 24.913 | 79.795 | 1.00 | 56.37 | AAAA | C |
| ATOH | 2229 | O | PRO | 232 | 41.498 | 25.492 | 79.137 | 1.00 | 55.79 | AAAA | O |
| ATOH | 2230 | H | ALA | 233 | 43.615 | 25.400 | 79.901 | 1.00 | 54.76 | AAAA | N |
| ATOH | 2232 | CA | ALA | 233 | 43.998 | 26.569 | 79.124 | 1.00 | 49.93 | AAAA | C |
| ATOH | 2233 | CB | ALA | 233 | 43.440 | 27.907 | 79.746 | 1.00 | 35.43 | AAAA | C |
| ATOH | 2234 | C | ALA | 233 | 45.502 | 26.662 | 79.974 | 1.00 | 49.79 | AAAA | C |
| ATOH | 2235 | O | ALA | 233 | 46.195 | 25.879 | 79.616 | 1.00 | 51.41 | AAAA | O |
| ATOH | 2236 | H | CYS | 234 | 45.984 | 27.508 | 78.072 | 1.00 | 45.07 | AAAA | N |
| ATOH | 2238 | CA | CYS | 234 | 47.430 | 27.518 | 77.907 | 1.00 | 48.63 | AAAA | C |
| ATOH | 2239 | C | CYS | 234 | 48.001 | 28.340 | 79.076 | 1.00 | 50.93 | AAAA | C |
| ATOH | 2240 | O | CYS | 234 | 47.650 | 29.513 | 79.250 | 1.00 | 47.57 | AAAA | O |
| ATOH | 2241 | CB | CYS | 234 | 47.816 | 28.034 | 76.511 | 1.00 | 43.10 | AAAA | C |
| ATOH | 2242 | SG | CYS | 234 | 47.608 | 26.789 | 75.226 | 1.00 | 43.04 | AAAA | S |
| ATOH | 2243 | H | PRO | 235 | 49.127 | 27.853 | 79.599 | 1.00 | 49.55 | AAAA | N |
| ATOH | 2244 | CD | PRO | 235 | 49.692 | 26.557 | 79.207 | 1.00 | 48.75 | AAAA | C |
| ATOH | 2245 | CA | PRO | 235 | 49.911 | 28.569 | 80.599 | 1.00 | 51.69 | AAAA | C |
| ATOH | 2246 | CB | PRO | 235 | 50.984 | 27.581 | 80.975 | 1.00 | 50.80 | AAAA | C |
| ATOH | 2247 | CG | PRO | 235 | 50.912 | 26.417 | 80.077 | 1.00 | 50.06 | AAAA | C |
| ATOH | 2249 | C | PRO | 235 | 50.487 | 29.852 | 80.050 | 1.00 | 57.11 | AAAA | C |
| ATOH | 2249 | O | PRO | 235 | 50.848 | 29.957 | 78.870 | 1.00 | 59.60 | AAAA | O |
| ATOH | 2250 | H | PRO | 236 | 50.676 | 30.875 | 80.887 | 1.00 | 59.95 | AAAA | N |
| ATOH | 2251 | CD | PRO | 236 | 50.405 | 30.822 | 82.363 | 1.00 | 55.85 | AAAA | C |
| ATOH | 2252 | CA | PRO | 236 | 51.323 | 32.143 | 80.493 | 1.00 | 52.27 | AAAA | C |
| ATOH | 2253 | CB | PRO | 236 | 51.695 | 32.814 | 81.826 | 1.00 | 53.62 | AAAA | C |
| ATOH | 2254 | CG | PRO | 236 | 50.652 | 32.277 | 82.754 | 1.00 | 56.73 | AAAA | C |
| ATOH | 2255 | C | PRO | 236 | 52.545 | 31.886 | 79.671 | 1.00 | 44.21 | AAAA | C |
| ATOH | 2256 | O | PRO | 236 | 53.218 | 30.892 | 79.928 | 1.00 | 43.40 | AAAA | O |
| ATOH | 2257 | H | ASN | 237 | 52.837 | 32.757 | 78.716 | 1.00 | 46.54 | AAAA | N |
| ATOH | 2259 | CA | ASN | 237 | 53.895 | 32.623 | 77.716 | 1.00 | 45.94 | AAAA | C |
| ATOH | 2260 | CB | ASN | 237 | 55.258 | 32.653 | 78.456 | 1.00 | 58.65 | AAAA | C |
| ATOH | 2261 | CG | ASN | 237 | 55.357 | 33.855 | 79.371 | 1.00 | 58.51 | AAAA | C |
| ATOH | 2262 | OD1 | ASN | 237 | 56.044 | 33.783 | 80.379 | 1.00 | 72.25 | AAAA | O |
| ATOH | 2263 | HD2 | ASN | 237 | 54.631 | 34.910 | 79.051 | 1.00 | 62.99 | AAAA | N |
| ATOH | 2266 | C | ASN | 237 | 53.897 | 31.425 | 76.788 | 1.00 | 46.87 | AAAA | C |
| ATOH | 2267 | O | ASN | 237 | 54.962 | 30.935 | 76.326 | 1.00 | 54.50 | AAAA | O |
| ATOH | 2268 | N | THR | 238 | 52.817 | 30.657 | 76.692 | 1.00 | 42.91 | AAAA | N |
| ATOH | 2270 | CA | THR | 238 | 52.617 | 29.567 | 75.780 | 1.00 | 40.20 | AAAA | C |
| ATOH | 2271 | CB | THR | 238 | 52.461 | 28.248 | 76.466 | 1.00 | 42.62 | AAAA | C |
| ATOH | 2272 | OG1 | THR | 238 | 51.227 | 28.343 | 77.237 | 1.00 | 50.89 | AAAA | O |
| ATOH | 2274 | CG2 | THR | 238 | 53.552 | 27.886 | 77.424 | 1.00 | 34.84 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 2275 | C | THR | 238 | 51.278 | 29.875 | 75.078 | 1.00 | 42.59 | AAAA | C |
| ATOH | 2276 | C | THR | 238 | 50.669 | 30.864 | 75.509 | 1.00 | 42.51 | AAAA | O |
| ATOH | 2277 | H | TYR | 239 | 51.051 | 29.488 | 73.832 | 1.00 | 42.62 | AAAA | H |
| ATOH | 2279 | CA | TYR | 239 | 49.949 | 29.959 | 73.024 | 1.00 | 41.87 | AAAA | C |
| ATOH | 2280 | CB | TYR | 239 | 50.457 | 30.907 | 71.931 | 1.00 | 44.86 | AAAA | C |
| ATOH | 2281 | CG | TYR | 239 | 51.099 | 32.125 | 72.564 | 1.00 | 42.05 | AAAA | C |
| ATOH | 2282 | CD1 | TYR | 239 | 52.467 | 32.086 | 72.815 | 1.00 | 39.41 | AAAA | C |
| ATOH | 2283 | CE1 | TYR | 239 | 53.092 | 33.152 | 73.415 | 1.00 | 43.27 | AAAA | C |
| ATOH | 2284 | CD2 | TYR | 239 | 50.376 | 33.230 | 72.923 | 1.00 | 44.15 | AAAA | C |
| ATOH | 2285 | CE2 | TYR | 239 | 50.972 | 34.310 | 73.536 | 1.00 | 46.22 | AAAA | C |
| ATOH | 2286 | CG | TYR | 239 | 52.339 | 34.243 | 73.779 | 1.00 | 50.49 | AAAA | C |
| ATOH | 2287 | OH | TYR | 239 | 53.013 | 35.289 | 74.387 | 1.00 | 55.47 | AAAA | O |
| ATOH | 2289 | C | TYR | 239 | 49.232 | 28.813 | 72.315 | 1.00 | 45.54 | AAAA | C |
| ATOH | 2290 | O | TYR | 239 | 49.922 | 27.810 | 72.021 | 1.00 | 46.66 | AAAA | O |
| ATOH | 2291 | H | ARG | 240 | 47.895 | 28.990 | 72.126 | 1.00 | 40.62 | AAAA | N |
| ATOH | 2293 | CA | ARG | 240 | 47.177 | 27.892 | 71.426 | 1.00 | 38.78 | AAAA | C |
| ATOH | 2294 | CB | ARG | 240 | 45.675 | 28.127 | 71.452 | 1.00 | 39.77 | AAAA | C |
| ATOH | 2295 | CG | ARG | 240 | 45.116 | 28.944 | 72.588 | 1.00 | 43.37 | AAAA | C |
| ATOH | 2296 | CD | ARG | 240 | 43.573 | 28.957 | 72.683 | 1.00 | 38.60 | AAAA | C |
| ATOH | 2297 | HE | ARG | 240 | 43.114 | 29.683 | 71.455 | 1.00 | 53.98 | AAAA | H |
| ATOH | 2299 | CG | ARG | 240 | 43.123 | 31.015 | 71.530 | 1.00 | 48.07 | AAAA | C |
| ATOH | 2300 | NH1 | ARG | 240 | 43.513 | 31.562 | 72.668 | 1.00 | 47.65 | AAAA | H |
| ATOH | 2303 | NH2 | ARG | 240 | 42.788 | 31.778 | 70.533 | 1.00 | 51.03 | AAAA | H |
| ATOH | 2306 | C | ARG | 240 | 47.627 | 27.737 | 69.979 | 1.00 | 31.72 | AAAA | C |
| ATOH | 2307 | O | ARG | 240 | 47.937 | 28.730 | 69.302 | 1.00 | 32.37 | AAAA | O |
| ATOH | 2308 | H | PHE | 241 | 47.779 | 26.542 | 69.549 | 1.00 | 27.95 | AAAA | N |
| ATOH | 2310 | CA | PHE | 241 | 49.182 | 26.269 | 68.183 | 1.00 | 30.41 | AAAA | C |
| ATOH | 2311 | CB | PHE | 241 | 49.678 | 25.940 | 68.151 | 1.00 | 34.83 | AAAA | C |
| ATOH | 2312 | CG | PHE | 241 | 50.235 | 25.653 | 66.773 | 1.00 | 26.84 | AAAA | C |
| ATOH | 2313 | CD1 | PHE | 241 | 50.165 | 26.567 | 65.753 | 1.00 | 25.31 | AAAA | C |
| ATOH | 2314 | CD2 | PHE | 241 | 50.785 | 24.417 | 66.573 | 1.00 | 27.38 | AAAA | C |
| ATOH | 2315 | CE1 | PHE | 241 | 50.676 | 26.232 | 64.509 | 1.00 | 37.24 | AAAA | C |
| ATOH | 2316 | CE2 | PHE | 241 | 51.294 | 24.101 | 65.320 | 1.00 | 38.45 | AAAA | C |
| ATOH | 2317 | CG | PHE | 241 | 51.281 | 25.010 | 64.281 | 1.00 | 21.17 | AAAA | C |
| ATOH | 2318 | C | PHE | 241 | 47.382 | 25.089 | 67.621 | 1.00 | 35.77 | AAAA | C |
| ATOH | 2319 | O | PHE | 241 | 47.543 | 24.013 | 68.186 | 1.00 | 36.77 | AAAA | O |
| ATOH | 2320 | H | GLU | 242 | 46.739 | 25.301 | 66.468 | 1.00 | 32.30 | AAAA | H |
| ATOH | 2322 | CA | GLU | 242 | 45.964 | 24.269 | 65.805 | 1.00 | 35.43 | AAAA | C |
| ATOH | 2323 | CB | GLU | 242 | 46.953 | 23.144 | 65.472 | 1.00 | 37.98 | AAAA | C |
| ATOH | 2324 | CG | GLU | 242 | 47.867 | 23.415 | 64.314 | 1.00 | 39.63 | AAAA | C |
| ATOH | 2325 | CD | GLU | 242 | 47.207 | 23.965 | 63.075 | 1.00 | 39.27 | AAAA | C |
| ATOH | 2326 | CE1 | GLU | 242 | 46.380 | 23.205 | 62.517 | 1.00 | 42.79 | AAAA | O |
| ATOH | 2327 | CE2 | GLU | 242 | 47.354 | 25.109 | 62.626 | 1.00 | 36.36 | AAAA | O |
| ATOH | 2328 | C | GLU | 242 | 44.752 | 23.771 | 66.600 | 1.00 | 34.36 | AAAA | C |
| ATOH | 2329 | O | GLU | 242 | 44.399 | 22.611 | 66.511 | 1.00 | 28.53 | AAAA | O |
| ATOH | 2330 | H | GLY | 243 | 44.135 | 24.589 | 67.449 | 1.00 | 36.94 | AAAA | H |
| ATOH | 2332 | CA | GLY | 243 | 43.048 | 24.154 | 68.303 | 1.00 | 34.57 | AAAA | C |
| ATOH | 2333 | C | GLY | 243 | 43.428 | 23.107 | 69.319 | 1.00 | 37.76 | AAAA | C |
| ATOH | 2334 | O | GLY | 243 | 42.474 | 22.473 | 69.746 | 1.00 | 43.00 | AAAA | O |
| ATOH | 2335 | H | TRP | 244 | 44.637 | 22.636 | 69.611 | 1.00 | 39.53 | AAAA | H |
| ATOH | 2337 | CA | TRP | 244 | 44.797 | 21.536 | 70.566 | 1.00 | 40.85 | AAAA | C |
| ATOH | 2338 | CB | TRP | 244 | 44.774 | 20.271 | 69.764 | 1.00 | 26.76 | AAAA | C |
| ATOH | 2339 | CG | TRP | 244 | 46.012 | 19.885 | 69.028 | 1.00 | 43.19 | AAAA | C |
| ATOH | 2340 | CD2 | TRP | 244 | 47.019 | 18.983 | 69.498 | 1.00 | 39.55 | AAAA | C |
| ATOH | 2341 | CE2 | TRP | 244 | 47.998 | 18.906 | 68.489 | 1.00 | 36.50 | AAAA | C |
| ATOH | 2342 | CE3 | TRP | 244 | 47.186 | 18.254 | 70.692 | 1.00 | 32.19 | AAAA | C |
| ATOH | 2343 | CD1 | TRP | 244 | 46.424 | 20.308 | 67.779 | 1.00 | 43.37 | AAAA | C |
| ATOH | 2344 | HE1 | TRP | 244 | 47.595 | 19.727 | 67.469 | 1.00 | 38.89 | AAAA | H |
| ATOH | 2346 | CE2 | TRP | 244 | 49.150 | 18.128 | 68.620 | 1.00 | 39.01 | AAAA | C |
| ATOH | 2347 | CE3 | TRP | 244 | 48.336 | 17.478 | 70.815 | 1.00 | 43.98 | AAAA | C |
| ATOH | 2348 | CH2 | TRP | 244 | 49.322 | 17.425 | 69.784 | 1.00 | 42.50 | AAAA | C |
| ATOH | 2349 | C | TRP | 244 | 45.998 | 21.517 | 71.509 | 1.00 | 42.98 | AAAA | C |
| ATOH | 2350 | O | TRP | 244 | 46.253 | 20.501 | 72.146 | 1.00 | 42.70 | AAAA | O |
| ATOH | 2351 | H | ARG | 245 | 46.888 | 22.485 | 71.435 | 1.00 | 44.16 | AAAA | H |
| ATOH | 2353 | CA | ARG | 245 | 48.168 | 22.472 | 72.095 | 1.00 | 46.47 | AAAA | C |
| ATOH | 2354 | CB | ARG | 245 | 49.203 | 21.602 | 71.367 | 1.00 | 47.30 | AAAA | C |
| ATOH | 2355 | CG | ARG | 245 | 49.885 | 22.309 | 70.203 | 1.00 | 48.97 | AAAA | C |
| ATOH | 2356 | CD | ARG | 245 | 51.129 | 21.552 | 69.819 | 1.00 | 39.28 | AAAA | C |
| ATOH | 2357 | HE | ARG | 245 | 51.586 | 21.665 | 68.444 | 1.00 | 50.96 | AAAA | H |
| ATOH | 2359 | CZ | ARG | 245 | 52.629 | 21.044 | 67.895 | 1.00 | 46.73 | AAAA | C |
| ATOH | 2360 | NH1 | ARG | 245 | 53.344 | 20.236 | 68.653 | 1.00 | 50.15 | AAAA | N |
| ATOH | 2363 | NH2 | ARG | 245 | 53.072 | 21.126 | 66.638 | 1.00 | 41.69 | AAAA | H |
| ATOH | 2366 | C | ARG | 245 | 48.771 | 23.963 | 72.271 | 1.00 | 46.01 | AAAA | C |
| ATOH | 2367 | O | ARG | 245 | 48.394 | 24.793 | 71.541 | 1.00 | 47.44 | AAAA | O |
| ATOH | 2368 | H | CYS | 246 | 49.625 | 23.881 | 73.317 | 1.00 | 42.08 | AAAA | H |
| ATOH | 2370 | CA | CYS | 246 | 50.246 | 25.199 | 73.628 | 1.00 | 43.48 | AAAA | C |
| ATOH | 2371 | C | CYS | 246 | 51.695 | 25.217 | 73.183 | 1.00 | 43.38 | AAAA | C |
| ATOH | 2372 | O | CYS | 246 | 52.476 | 24.239 | 73.320 | 1.00 | 42.51 | AAAA | O |
| ATOH | 2373 | CB | CYS | 246 | 50.102 | 25.392 | 75.138 | 1.00 | 48.91 | AAAA | C |
| ATOH | 2374 | SG | CYS | 246 | 48.386 | 25.049 | 75.797 | 1.00 | 43.68 | AAAA | S |
| ATOH | 2375 | H | VAL | 247 | 52.121 | 26.288 | 72.564 | 1.00 | 41.21 | AAAA | N |
| ATOH | 2377 | CA | VAL | 247 | 53.417 | 26.468 | 71.982 | 1.00 | 36.51 | AAAA | C |
| ATOH | 2378 | CB | VAL | 247 | 53.568 | 26.357 | 70.444 | 1.00 | 36.87 | AAAA | C |
| ATOH | 2379 | CG1 | VAL | 247 | 53.089 | 24.988 | 70.024 | 1.00 | 32.71 | AAAA | C |
| ATOH | 2380 | CG2 | VAL | 247 | 53.129 | 27.602 | 69.729 | 1.00 | 28.20 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 2391 | " | VAL | 247 | 53.969 | 27.812 | 72.373 | 1.00 | 39.37 | AAAA | C |
| ATOM | 2392 | " | VAL | 247 | 53.230 | 29.770 | 72.540 | 1.00 | 38.80 | AAAA | O |
| ATOM | 2393 | " | ASP | 248 | 55.291 | 27.820 | 72.711 | 1.00 | 45.21 | AAAA | N |
| ATOM | 2395 | CA | ASF | 248 | 55.895 | 29.115 | 73.098 | 1.00 | 40.19 | AAAA | C |
| ATOM | 2396 | CB | ASP | 248 | 57.091 | 28.946 | 73.953 | 1.00 | 42.63 | AAAA | C |
| ATOM | 2397 | CG | ASP | 248 | 58.126 | 27.997 | 73.394 | 1.00 | 58.81 | AAAA | C |
| ATOM | 2398 | OD1 | ASF | 248 | 59.067 | 27.795 | 74.187 | 1.00 | 53.06 | AAAA | O |
| ATOM | 2399 | OD2 | ASF | 248 | 58.167 | 27.395 | 72.313 | 1.00 | 69.51 | AAAA | O |
| ATOM | 2399 | C | ASP | 248 | 56.315 | 29.883 | 71.839 | 1.00 | 36.99 | AAAA | C |
| ATOM | 2391 | O | ASF | 248 | 56.292 | 29.288 | 70.772 | 1.00 | 39.70 | AAAA | O |
| ATOM | 2392 | " | ARG | 249 | 56.545 | 31.163 | 71.918 | 1.00 | 30.72 | AAAA | H |
| ATOM | 2394 | CA | ARG | 249 | 56.950 | 32.057 | 70.906 | 1.00 | 36.17 | AAAA | C |
| ATOM | 2395 | CB | ARG | 249 | 57.223 | 33.485 | 71.491 | 1.00 | 21.29 | AAAA | C |
| ATOM | 2396 | CG | ARG | 249 | 57.594 | 34.424 | 70.326 | 1.00 | 24.96 | AAAA | C |
| ATOM | 2397 | CD | ARG | 249 | 57.814 | 35.811 | 70.843 | 1.00 | 21.23 | AAAA | C |
| ATOM | 2398 | HE | ARG | 249 | 56.658 | 36.150 | 71.689 | 1.00 | 39.75 | AAAA | N |
| ATOM | 2400 | CG | ARG | 249 | 55.632 | 36.823 | 71.101 | 1.00 | 39.35 | AAAA | C |
| ATOM | 2401 | NH1 | ARG | 249 | 55.642 | 37.118 | 69.801 | 1.00 | 25.41 | AAAA | H |
| ATOM | 2404 | NH2 | ARG | 249 | 54.641 | 37.118 | 71.946 | 1.00 | 44.04 | AAAA | H |
| ATOM | 2407 | C | ARG | 249 | 58.134 | 31.685 | 70.010 | 1.00 | 40.63 | AAAA | C |
| ATOM | 2408 | O | ARG | 249 | 58.086 | 31.923 | 68.797 | 1.00 | 44.79 | AAAA | O |
| ATOM | 2409 | " | ASP | 250 | 59.149 | 30.974 | 70.468 | 1.00 | 41.87 | AAAA | H |
| ATOM | 2411 | CA | ASP | 250 | 60.287 | 30.739 | 69.606 | 1.00 | 46.90 | AAAA | C |
| ATOM | 2412 | CB | ASP | 250 | 61.740 | 30.726 | 70.154 | 1.00 | 53.11 | AAAA | C |
| ATOM | 2413 | CG | ASP | 250 | 62.421 | 32.122 | 70.081 | 1.00 | 71.49 | AAAA | C |
| ATOM | 2414 | OD1 | ASP | 250 | 63.124 | 32.682 | 69.176 | 1.00 | 58.53 | AAAA | O |
| ATOM | 2415 | OD2 | ASP | 250 | 62.272 | 32.928 | 71.071 | 1.00 | 70.30 | AAAA | O |
| ATOM | 2416 | C | ASP | 250 | 59.881 | 29.536 | 68.771 | 1.00 | 41.22 | AAAA | C |
| ATOM | 2417 | O | ASP | 250 | 60.291 | 29.443 | 67.616 | 1.00 | 39.06 | AAAA | O |
| ATOM | 2418 | " | PHE | 251 | 59.116 | 28.609 | 69.299 | 1.00 | 36.13 | AAAA | H |
| ATOM | 2420 | CA | PHE | 251 | 58.457 | 27.601 | 68.489 | 1.00 | 34.88 | AAAA | C |
| ATOM | 2421 | CB | PHE | 251 | 57.468 | 26.746 | 69.256 | 1.00 | 29.82 | AAAA | C |
| ATOM | 2422 | CG | PHE | 251 | 56.701 | 25.801 | 68.385 | 1.00 | 41.50 | AAAA | C |
| ATOM | 2423 | CD1 | PHE | 251 | 57.101 | 24.479 | 68.263 | 1.00 | 30.66 | AAAA | C |
| ATOM | 2424 | CD2 | PHE | 251 | 55.559 | 26.213 | 67.686 | 1.00 | 37.78 | AAAA | C |
| ATOM | 2425 | CE1 | PHE | 251 | 56.414 | 23.597 | 67.424 | 1.00 | 29.30 | AAAA | C |
| ATOM | 2426 | CE2 | PHE | 251 | 54.847 | 25.372 | 66.856 | 1.00 | 36.09 | AAAA | C |
| ATOM | 2427 | CC | PHE | 251 | 55.294 | 24.070 | 66.715 | 1.00 | 36.21 | AAAA | C |
| ATOM | 2428 | C | PHE | 251 | 57.624 | 28.290 | 67.338 | 1.00 | 39.28 | AAAA | C |
| ATOM | 2429 | O | PHE | 251 | 57.911 | 29.010 | 66.144 | 1.00 | 30.27 | AAAA | O |
| ATOM | 2430 | " | CYS | 252 | 56.734 | 29.225 | 67.713 | 1.00 | 35.13 | AAAA | H |
| ATOM | 2432 | CA | CYS | 252 | 55.895 | 29.870 | 66.728 | 1.00 | 38.80 | AAAA | C |
| ATOM | 2433 | C | CYS | 252 | 56.827 | 30.599 | 65.747 | 1.00 | 44.73 | AAAA | C |
| ATOM | 2434 | O | CYS | 252 | 56.552 | 30.534 | 64.536 | 1.00 | 43.20 | AAAA | O |
| ATOM | 2435 | CB | CYS | 252 | 54.903 | 30.778 | 67.379 | 1.00 | 35.65 | AAAA | C |
| ATOM | 2436 | SG | CYS | 252 | 53.562 | 31.544 | 66.459 | 1.00 | 39.03 | AAAA | S |
| ATOM | 2437 | " | ALA | 253 | 57.872 | 31.256 | 66.285 | 1.00 | 41.53 | AAAA | H |
| ATOM | 2439 | CA | ALA | 253 | 58.687 | 32.071 | 65.415 | 1.00 | 40.39 | AAAA | C |
| ATOM | 2440 | CB | ALA | 253 | 59.529 | 33.098 | 66.172 | 1.00 | 36.07 | AAAA | C |
| ATOM | 2441 | C | ALA | 253 | 59.551 | 31.167 | 64.539 | 1.00 | 42.89 | AAAA | C |
| ATOM | 2442 | O | ALA | 253 | 60.147 | 31.735 | 63.640 | 1.00 | 47.42 | AAAA | O |
| ATOM | 2443 | " | ASU | 254 | 59.657 | 29.859 | 64.700 | 1.00 | 38.75 | AAAA | H |
| ATOM | 2445 | CA | ASU | 254 | 60.546 | 29.073 | 63.928 | 1.00 | 42.94 | AAAA | C |
| ATOM | 2446 | CB | ASU | 254 | 61.667 | 29.497 | 64.847 | 1.00 | 48.09 | AAAA | C |
| ATOM | 2447 | CG | ASU | 254 | 62.696 | 29.635 | 65.031 | 1.00 | 49.54 | AAAA | C |
| ATOM | 2448 | OD1 | ASU | 254 | 63.468 | 29.840 | 64.081 | 1.00 | 61.38 | AAAA | O |
| ATOM | 2449 | HD2 | ASU | 254 | 62.607 | 30.321 | 66.144 | 1.00 | 48.38 | AAAA | N |
| ATOM | 2452 | C | ASN | 254 | 59.907 | 27.959 | 63.135 | 1.00 | 53.72 | AAAA | C |
| ATOM | 2453 | O | ASN | 254 | 60.552 | 26.965 | 62.804 | 1.00 | 51.19 | AAAA | O |
| ATOM | 2454 | " | ILE | 255 | 58.612 | 28.136 | 62.766 | 1.00 | 57.77 | AAAA | N |
| ATOM | 2456 | CA | ILE | 255 | 57.828 | 27.107 | 62.134 | 1.00 | 53.29 | AAAA | C |
| ATOM | 2457 | CB | ILE | 255 | 56.329 | 27.322 | 62.304 | 1.00 | 50.41 | AAAA | C |
| ATOM | 2458 | CG2 | ILE | 255 | 55.477 | 26.595 | 61.246 | 1.00 | 51.95 | AAAA | C |
| ATOM | 2459 | CG1 | ILE | 255 | 55.778 | 26.675 | 63.553 | 1.00 | 40.59 | AAAA | C |
| ATOM | 2460 | CD1 | ILE | 255 | 54.479 | 27.317 | 64.006 | 1.00 | 38.97 | AAAA | C |
| ATOM | 2461 | C | ILE | 255 | 58.127 | 26.886 | 60.651 | 1.00 | 52.62 | AAAA | C |
| ATOM | 2462 | O | ILE | 255 | 58.196 | 25.709 | 60.252 | 1.00 | 53.96 | AAAA | O |
| ATOM | 2463 | " | LEU | 256 | 58.290 | 27.960 | 59.918 | 1.00 | 49.96 | AAAA | N |
| ATOM | 2465 | CA | LEU | 256 | 58.680 | 27.764 | 58.516 | 1.00 | 63.68 | AAAA | C |
| ATOM | 2466 | CB | LEU | 256 | 58.175 | 29.012 | 57.799 | 1.00 | 56.80 | AAAA | C |
| ATOM | 2467 | CG | LEU | 256 | 56.671 | 29.196 | 57.864 | 1.00 | 59.11 | AAAA | C |
| ATOM | 2468 | CD1 | LEU | 256 | 56.310 | 30.654 | 57.645 | 1.00 | 43.31 | AAAA | C |
| ATOM | 2469 | CD2 | LEU | 256 | 55.965 | 28.222 | 56.928 | 1.00 | 55.88 | AAAA | C |
| ATOM | 2470 | C | LEU | 256 | 60.193 | 27.622 | 58.355 | 1.00 | 66.23 | AAAA | C |
| ATOM | 2471 | O | LEU | 256 | 60.691 | 27.511 | 57.245 | 1.00 | 70.29 | AAAA | O |
| ATOM | 2472 | " | SER | 257 | 60.942 | 27.559 | 59.430 | 1.00 | 64.61 | AAAA | N |
| ATOM | 2474 | CA | SER | 257 | 62.352 | 27.529 | 59.534 | 1.00 | 69.23 | AAAA | C |
| ATOM | 2475 | CB | SER | 257 | 62.924 | 27.318 | 60.955 | 1.00 | 62.45 | AAAA | C |
| ATOM | 2476 | OG | SER | 257 | 63.381 | 25.980 | 61.074 | 1.00 | 56.18 | AAAA | O |
| ATOM | 2478 | C | SER | 257 | 62.973 | 26.497 | 58.610 | 1.00 | 70.77 | AAAA | C |
| ATOM | 2479 | O | SER | 257 | 64.127 | 26.731 | 58.246 | 1.00 | 72.50 | AAAA | O |
| ATOM | 2480 | " | ALA | 258 | 62.322 | 25.389 | 58.320 | 1.00 | 74.61 | AAAA | N |
| ATOM | 2482 | CA | ALA | 258 | 62.933 | 24.498 | 57.343 | 1.00 | 76.34 | AAAA | C |
| ATOM | 2483 | CB | ALA | 258 | 62.570 | 23.039 | 57.584 | 1.00 | 80.82 | AAAA | C |
| ATOM | 2484 | C | ALA | 258 | 62.663 | 24.964 | 55.921 | 1.00 | 78.21 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|--------|------|---|
| ATOM | 2485 | O | ALA | 258 | 62.880 | 24.139 | 55.029 | 1.00 | 79.60 | AAAA | O |
| ATOM | 2486 | H | GLU | 259 | 62.069 | 26.109 | 55.651 | 1.00 | 79.05 | AAAA | H |
| ATOM | 2488 | CA | GLU | 259 | 61.742 | 26.621 | 54.349 | 1.00 | 83.84 | AAAA | C |
| ATOM | 2489 | CB | GLU | 259 | 60.226 | 26.457 | 54.135 | 1.00 | 86.99 | AAAA | C |
| ATOM | 2490 | CG | GLU | 259 | 59.687 | 25.049 | 54.314 | 1.00 | 89.38 | AAAA | C |
| ATOM | 2491 | CD | GLU | 259 | 58.364 | 25.032 | 55.057 | 1.00 | 97.77 | AAAA | C |
| ATOM | 2492 | OE1 | GLU | 259 | 58.080 | 24.088 | 55.838 | 1.00 | 101.45 | AAAA | O |
| ATOM | 2493 | OE2 | GLU | 259 | 57.598 | 26.002 | 54.837 | 1.00 | 94.58 | AAAA | O |
| ATOM | 2494 | C | GLU | 259 | 62.117 | 28.078 | 54.083 | 1.00 | 85.43 | AAAA | C |
| ATOM | 2495 | O | GLU | 259 | 62.059 | 29.009 | 54.903 | 1.00 | 88.01 | AAAA | O |
| ATOM | 2496 | H | SER | 260 | 62.298 | 28.338 | 52.799 | 1.00 | 84.66 | AAAA | H |
| ATOM | 2499 | CA | SER | 260 | 62.725 | 29.625 | 52.254 | 1.00 | 84.03 | AAAA | C |
| ATOM | 2499 | CB | SER | 260 | 63.753 | 29.269 | 51.173 | 1.00 | 87.24 | AAAA | C |
| ATOM | 2500 | CG | SER | 260 | 63.306 | 29.419 | 49.835 | 1.00 | 93.65 | AAAA | O |
| ATOM | 2502 | C | SER | 260 | 61.558 | 30.466 | 51.789 | 1.00 | 80.84 | AAAA | C |
| ATOM | 2503 | O | SER | 260 | 61.496 | 30.889 | 50.635 | 1.00 | 81.31 | AAAA | O |
| ATOM | 2504 | H | SER | 261 | 60.617 | 30.785 | 52.685 | 1.00 | 78.56 | AAAA | H |
| ATOM | 2506 | CA | SER | 261 | 59.423 | 31.540 | 52.308 | 1.00 | 72.13 | AAAA | C |
| ATOM | 2507 | CB | SER | 261 | 58.179 | 31.297 | 53.170 | 1.00 | 67.30 | AAAA | C |
| ATOM | 2508 | CG | SER | 261 | 57.436 | 30.334 | 52.451 | 1.00 | 74.74 | AAAA | O |
| ATOM | 2510 | C | SER | 261 | 59.683 | 33.032 | 52.318 | 1.00 | 66.90 | AAAA | C |
| ATOM | 2511 | O | SER | 261 | 60.048 | 33.588 | 53.334 | 1.00 | 63.24 | AAAA | O |
| ATOM | 2512 | H | ASP | 262 | 59.364 | 33.659 | 51.204 | 1.00 | 65.30 | AAAA | H |
| ATOM | 2514 | CA | ASP | 262 | 59.358 | 35.071 | 50.915 | 1.00 | 58.55 | AAAA | C |
| ATOM | 2515 | CB | ASP | 262 | 59.268 | 35.285 | 49.400 | 1.00 | 64.85 | AAAA | C |
| ATOM | 2516 | CG | ASP | 262 | 59.389 | 36.713 | 48.931 | 1.00 | 76.42 | AAAA | C |
| ATOM | 2517 | OD1 | ASP | 262 | 59.473 | 37.708 | 49.701 | 1.00 | 79.81 | AAAA | O |
| ATOM | 2518 | OD2 | ASP | 262 | 59.404 | 36.873 | 47.671 | 1.00 | 80.46 | AAAA | O |
| ATOM | 2519 | C | ASP | 262 | 58.121 | 35.706 | 51.529 | 1.00 | 56.88 | AAAA | C |
| ATOM | 2520 | O | ASP | 262 | 57.851 | 36.918 | 51.510 | 1.00 | 52.48 | AAAA | O |
| ATOM | 2521 | H | SER | 263 | 57.259 | 34.849 | 52.118 | 1.00 | 53.43 | AAAA | H |
| ATOM | 2523 | CA | SER | 263 | 56.047 | 35.352 | 52.734 | 1.00 | 52.84 | AAAA | C |
| ATOM | 2524 | CB | SER | 263 | 55.020 | 34.245 | 52.885 | 1.00 | 46.60 | AAAA | C |
| ATOM | 2525 | CG | SER | 263 | 55.149 | 33.348 | 51.791 | 1.00 | 66.80 | AAAA | O |
| ATOM | 2527 | C | SER | 263 | 56.310 | 35.965 | 54.117 | 1.00 | 49.52 | AAAA | C |
| ATOM | 2529 | O | SER | 263 | 57.396 | 35.737 | 54.709 | 1.00 | 42.33 | AAAA | O |
| ATOM | 2529 | H | GLU | 264 | 55.320 | 36.793 | 54.540 | 1.00 | 38.93 | AAAA | H |
| ATOM | 2531 | CA | GLU | 264 | 55.362 | 37.022 | 55.921 | 1.00 | 36.70 | AAAA | C |
| ATOM | 2532 | CB | GLU | 264 | 54.359 | 39.337 | 56.208 | 1.00 | 43.71 | AAAA | C |
| ATOM | 2533 | CG | GLU | 264 | 54.575 | 39.492 | 55.219 | 1.00 | 37.74 | AAAA | C |
| ATOM | 2534 | CD | GLU | 264 | 55.374 | 40.632 | 55.793 | 1.00 | 34.36 | AAAA | C |
| ATOM | 2535 | CE1 | GLU | 264 | 55.493 | 41.600 | 57.034 | 1.00 | 41.55 | AAAA | O |
| ATOM | 2536 | CE2 | GLU | 264 | 55.832 | 41.576 | 55.146 | 1.00 | 39.60 | AAAA | O |
| ATOM | 2537 | C | GLU | 264 | 55.099 | 38.056 | 56.827 | 1.00 | 35.84 | AAAA | C |
| ATOM | 2539 | O | GLU | 264 | 54.368 | 38.151 | 56.355 | 1.00 | 39.60 | AAAA | O |
| ATOM | 2539 | H | GLY | 265 | 55.801 | 35.938 | 57.962 | 1.00 | 35.64 | AAAA | H |
| ATOM | 2541 | CA | GLY | 265 | 55.671 | 34.690 | 58.727 | 1.00 | 40.30 | AAAA | C |
| ATOM | 2542 | C | GLY | 265 | 54.622 | 34.716 | 59.829 | 1.00 | 39.51 | AAAA | C |
| ATOM | 2543 | O | GLY | 265 | 53.951 | 35.699 | 60.135 | 1.00 | 37.20 | AAAA | O |
| ATOM | 2544 | H | PHE | 266 | 54.537 | 33.569 | 60.516 | 1.00 | 35.75 | AAAA | H |
| ATOM | 2546 | CA | PHE | 266 | 53.637 | 33.434 | 61.625 | 1.00 | 33.70 | AAAA | C |
| ATOM | 2547 | CB | PHE | 266 | 53.924 | 32.155 | 62.386 | 1.00 | 28.20 | AAAA | C |
| ATOM | 2548 | CG | PHE | 266 | 53.356 | 30.958 | 61.671 | 1.00 | 37.07 | AAAA | C |
| ATOM | 2549 | CD1 | PHE | 266 | 53.760 | 30.618 | 60.377 | 1.00 | 34.72 | AAAA | C |
| ATOM | 2550 | CD2 | PHE | 266 | 52.383 | 30.185 | 62.313 | 1.00 | 25.65 | AAAA | C |
| ATOM | 2551 | CE1 | PHE | 266 | 53.225 | 29.506 | 59.760 | 1.00 | 37.72 | AAAA | C |
| ATOM | 2552 | CE2 | PHE | 266 | 51.879 | 29.094 | 61.672 | 1.00 | 24.63 | AAAA | C |
| ATOM | 2553 | CG | PHE | 266 | 52.260 | 29.708 | 60.402 | 1.00 | 23.58 | AAAA | C |
| ATOM | 2554 | C | PHE | 266 | 53.571 | 34.570 | 62.608 | 1.00 | 35.82 | AAAA | C |
| ATOM | 2555 | O | PHE | 266 | 54.446 | 35.372 | 62.879 | 1.00 | 39.23 | AAAA | O |
| ATOM | 2556 | H | VAL | 267 | 52.360 | 34.763 | 63.161 | 1.00 | 37.10 | AAAA | H |
| ATOM | 2558 | CA | VAL | 267 | 52.118 | 35.812 | 64.113 | 1.00 | 36.09 | AAAA | C |
| ATOM | 2559 | CB | VAL | 267 | 51.315 | 36.974 | 63.567 | 1.00 | 39.01 | AAAA | C |
| ATOM | 2560 | CG1 | VAL | 267 | 51.626 | 37.601 | 62.230 | 1.00 | 31.10 | AAAA | C |
| ATOM | 2561 | CG2 | VAL | 267 | 49.890 | 36.400 | 63.570 | 1.00 | 36.88 | AAAA | C |
| ATOM | 2562 | C | VAL | 267 | 51.506 | 35.260 | 65.400 | 1.00 | 33.55 | AAAA | C |
| ATOM | 2563 | O | VAL | 267 | 51.202 | 34.098 | 65.515 | 1.00 | 32.41 | AAAA | O |
| ATOM | 2564 | H | ILE | 268 | 51.539 | 36.088 | 66.477 | 1.00 | 35.88 | AAAA | H |
| ATOM | 2566 | CA | ILE | 268 | 50.867 | 35.573 | 67.691 | 1.00 | 39.79 | AAAA | C |
| ATOM | 2567 | CB | ILE | 268 | 51.791 | 35.232 | 68.849 | 1.00 | 31.17 | AAAA | C |
| ATOM | 2568 | CG2 | ILE | 268 | 50.922 | 35.253 | 70.150 | 1.00 | 32.66 | AAAA | C |
| ATOM | 2569 | CG1 | ILE | 268 | 52.403 | 33.966 | 68.724 | 1.00 | 23.56 | AAAA | C |
| ATOM | 2570 | CD1 | ILE | 268 | 53.421 | 33.546 | 69.806 | 1.00 | 25.93 | AAAA | C |
| ATOM | 2571 | C | ILE | 268 | 49.806 | 36.608 | 69.060 | 1.00 | 42.44 | AAAA | C |
| ATOM | 2572 | O | ILE | 268 | 50.116 | 37.767 | 68.327 | 1.00 | 39.99 | AAAA | O |
| ATOM | 2573 | H | HIS | 269 | 48.529 | 36.292 | 67.864 | 1.00 | 44.26 | AAAA | H |
| ATOM | 2575 | CA | HIS | 269 | 47.491 | 37.320 | 68.173 | 1.00 | 44.29 | AAAA | C |
| ATOM | 2576 | CB | HIS | 269 | 46.885 | 37.876 | 66.901 | 1.00 | 45.48 | AAAA | C |
| ATOM | 2577 | CG | HIS | 269 | 45.915 | 38.986 | 67.079 | 1.00 | 54.33 | AAAA | C |
| ATOM | 2578 | CD2 | HIS | 269 | 44.551 | 39.014 | 67.096 | 1.00 | 46.61 | AAAA | C |
| ATOM | 2579 | ND1 | HIS | 269 | 46.356 | 40.280 | 67.307 | 1.00 | 51.86 | AAAA | H |
| ATOM | 2581 | CE1 | HIS | 269 | 45.282 | 41.057 | 67.437 | 1.00 | 55.17 | AAAA | C |
| ATOM | 2582 | HE2 | HIS | 269 | 44.175 | 40.324 | 67.309 | 1.00 | 46.97 | AAAA | N |
| ATOM | 2584 | C | HIS | 269 | 46.423 | 36.740 | 69.074 | 1.00 | 45.54 | AAAA | C |
| ATOM | 2585 | O | HIS | 269 | 46.076 | 35.552 | 69.027 | 1.00 | 42.94 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|--------|-------|
| ATOH | 2586 | H | ASP | 270 | 45.952 | 37.526 | 70.059 | 1.00 | 43.82 |
| ATOH | 2588 | CA | ASP | 270 | 44.948 | 37.025 | 71.001 | 1.00 | 48.03 |
| ATOH | 2589 | CB | ASP | 270 | 43.573 | 37.014 | 70.338 | 1.00 | 63.63 |
| ATOH | 2590 | CG | ASP | 270 | 42.919 | 38.393 | 70.294 | 1.00 | 80.82 |
| ATOH | 2591 | OD1 | ASP | 270 | 41.737 | 38.379 | 69.835 | 1.00 | 90.92 |
| ATOH | 2592 | OD2 | ASP | 270 | 43.407 | 39.494 | 70.652 | 1.00 | 86.49 |
| ATOH | 2593 | C | ASP | 270 | 45.226 | 35.667 | 71.594 | 1.00 | 44.66 |
| ATOH | 2594 | O | ASP | 270 | 44.357 | 34.782 | 71.576 | 1.00 | 45.54 |
| ATOH | 2595 | H | GLY | 271 | 46.477 | 35.379 | 71.924 | 1.00 | 41.63 |
| ATOH | 2597 | CA | GLY | 271 | 46.839 | 34.117 | 72.506 | 1.00 | 37.20 |
| ATOH | 2598 | C | GLY | 271 | 46.818 | 32.998 | 71.537 | 1.00 | 39.15 |
| ATOH | 2599 | O | GLY | 271 | 46.775 | 31.865 | 72.039 | 1.00 | 46.56 |
| ATOH | 2600 | H | GLU | 272 | 47.015 | 33.292 | 70.251 | 1.00 | 41.49 |
| ATOH | 2602 | CA | GLU | 272 | 47.108 | 32.092 | 69.371 | 1.00 | 43.56 |
| ATOH | 2603 | CB | GLU | 272 | 45.752 | 31.737 | 68.876 | 1.00 | 37.58 |
| ATOH | 2604 | CG | GLU | 272 | 45.778 | 30.600 | 67.839 | 1.00 | 45.30 |
| ATOH | 2605 | CD | GLU | 272 | 44.413 | 30.528 | 67.149 | 1.00 | 36.92 |
| ATOH | 2606 | OE1 | GLU | 272 | 43.545 | 31.345 | 67.533 | 1.00 | 48.41 |
| ATOH | 2607 | OE2 | GLU | 272 | 44.223 | 29.696 | 66.286 | 1.00 | 44.10 |
| ATOH | 2608 | C | GLU | 272 | 48.211 | 32.324 | 68.335 | 1.00 | 40.32 |
| ATOH | 2609 | O | GLU | 272 | 48.445 | 33.447 | 67.896 | 1.00 | 37.04 |
| ATOH | 2610 | H | CYS | 273 | 48.942 | 31.237 | 68.138 | 1.00 | 38.83 |
| ATOH | 2612 | CA | CYS | 273 | 50.046 | 31.187 | 67.188 | 1.00 | 40.27 |
| ATOH | 2613 | C | CYS | 273 | 49.321 | 30.810 | 65.883 | 1.00 | 42.16 |
| ATOH | 2614 | O | CYS | 273 | 48.713 | 29.712 | 65.831 | 1.00 | 40.86 |
| ATOH | 2615 | CB | CYS | 273 | 51.098 | 30.148 | 67.529 | 1.00 | 40.21 |
| ATOH | 2616 | SG | CYS | 273 | 52.337 | 29.825 | 66.260 | 1.00 | 39.79 |
| ATOH | 2617 | H | MET | 274 | 49.373 | 31.749 | 64.933 | 1.00 | 33.70 |
| ATOH | 2619 | CA | MET | 274 | 48.586 | 31.351 | 63.720 | 1.00 | 36.68 |
| ATOH | 2620 | CB | MET | 274 | 47.136 | 31.861 | 63.847 | 1.00 | 29.11 |
| ATOH | 2621 | CG | MET | 274 | 46.923 | 33.379 | 63.691 | 1.00 | 36.51 |
| ATOH | 2622 | SD | MET | 274 | 45.477 | 33.921 | 64.677 | 1.00 | 40.00 |
| ATOH | 2623 | SE | MET | 274 | 45.659 | 35.658 | 64.754 | 1.00 | 22.47 |
| ATOH | 2624 | C | MET | 274 | 49.426 | 31.900 | 62.608 | 1.00 | 39.35 |
| ATOH | 2625 | O | MET | 274 | 50.167 | 32.880 | 62.672 | 1.00 | 41.00 |
| ATOH | 2626 | H | GLN | 275 | 49.378 | 31.353 | 61.428 | 1.00 | 42.55 |
| ATOH | 2628 | CA | GLN | 275 | 50.041 | 31.934 | 60.232 | 1.00 | 37.69 |
| ATOH | 2629 | CB | GLN | 275 | 49.619 | 30.765 | 59.242 | 1.00 | 34.01 |
| ATOH | 2630 | CG | GLN | 275 | 49.329 | 31.274 | 57.864 | 1.00 | 56.40 |
| ATOH | 2631 | CD | GLN | 275 | 49.275 | 30.190 | 56.812 | 1.00 | 66.46 |
| ATOH | 2632 | OE1 | GLN | 275 | 49.941 | 29.151 | 56.910 | 1.00 | 67.24 |
| ATOH | 2633 | OE2 | GLN | 275 | 48.451 | 30.436 | 55.799 | 1.00 | 78.29 |
| ATOH | 2636 | C | GLN | 275 | 49.721 | 33.195 | 59.720 | 1.00 | 35.41 |
| ATOH | 2637 | O | GLN | 275 | 50.526 | 33.831 | 59.064 | 1.00</ | |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 2685 | C | PHE | 281 | 45.630 | 43.217 | 60.240 | 1.00 | 48.00 | AAAA | C |
| ATOH | 2686 | O | PHE | 281 | 45.738 | 42.395 | 59.327 | 1.00 | 38.84 | AAAA | O |
| ATOH | 2687 | H | ILE | 282 | 46.570 | 43.990 | 60.557 | 1.00 | 49.55 | AAAA | H |
| ATOH | 2689 | CA | ILE | 282 | 47.907 | 43.984 | 59.748 | 1.00 | 45.00 | AAAA | C |
| ATOH | 2690 | CB | ILE | 282 | 47.945 | 45.198 | 58.799 | 1.00 | 30.25 | AAAA | C |
| ATOH | 2691 | CG2 | ILE | 282 | 48.041 | 46.494 | 59.507 | 1.00 | 24.60 | AAAA | C |
| ATOH | 2692 | CG1 | ILE | 282 | 49.092 | 45.022 | 57.795 | 1.00 | 38.71 | AAAA | C |
| ATOH | 2693 | CD1 | ILE | 282 | 49.194 | 46.643 | 56.669 | 1.00 | 33.38 | AAAA | C |
| ATOH | 2694 | C | ILE | 282 | 49.081 | 43.889 | 60.673 | 1.00 | 44.30 | AAAA | C |
| ATOH | 2695 | O | ILE | 282 | 49.078 | 44.447 | 61.759 | 1.00 | 48.49 | AAAA | O |
| ATOH | 2696 | H | ARG | 283 | 50.126 | 43.153 | 60.298 | 1.00 | 48.68 | AAAA | H |
| ATOH | 2698 | CA | ARG | 283 | 51.396 | 43.094 | 61.048 | 1.00 | 39.30 | AAAA | C |
| ATOH | 2699 | CB | ARG | 283 | 52.300 | 42.000 | 60.286 | 1.00 | 41.10 | AAAA | C |
| ATOH | 2700 | CG | ARG | 283 | 52.295 | 40.696 | 60.515 | 1.00 | 29.19 | AAAA | C |
| ATOH | 2701 | CD | ARG | 283 | 53.078 | 39.996 | 59.451 | 1.00 | 29.85 | AAAA | C |
| ATOH | 2702 | HE | ARG | 283 | 52.823 | 38.545 | 59.404 | 1.00 | 29.39 | AAAA | N |
| ATOH | 2704 | CE | ARG | 283 | 51.862 | 39.024 | 58.646 | 1.00 | 37.61 | AAAA | C |
| ATOH | 2705 | NH1 | ARG | 283 | 51.065 | 38.846 | 57.944 | 1.00 | 31.41 | AAAA | N |
| ATOH | 2708 | NH2 | ARG | 283 | 51.651 | 36.722 | 58.596 | 1.00 | 31.97 | AAAA | N |
| ATOH | 2711 | C | ARG | 283 | 51.945 | 44.498 | 61.190 | 1.00 | 42.27 | AAAA | C |
| ATOH | 2712 | O | ARG | 283 | 51.931 | 45.228 | 60.173 | 1.00 | 43.42 | AAAA | O |
| ATOH | 2713 | H | ASH | 284 | 52.362 | 44.886 | 62.422 | 1.00 | 39.49 | AAAA | N |
| ATOH | 2715 | CA | ASH | 284 | 52.733 | 46.311 | 62.574 | 1.00 | 42.07 | AAAA | C |
| ATOH | 2721 | C | ASH | 284 | 54.078 | 46.656 | 61.929 | 1.00 | 41.64 | AAAA | C |
| ATOH | 2722 | O | ASH | 284 | 54.431 | 47.798 | 61.742 | 1.00 | 39.01 | AAAA | O |
| ATOH | 2716 | CB | ASH | 284 | 52.734 | 46.760 | 64.032 | 1.00 | 37.33 | AAAA | C |
| ATOH | 2717 | CG | ASH | 284 | 53.917 | 46.028 | 64.611 | 1.00 | 50.21 | AAAA | C |
| ATOH | 2719 | OD1 | ASH | 284 | 54.609 | 45.104 | 64.192 | 1.00 | 44.30 | AAAA | O |
| ATOH | 2719 | HD2 | ASH | 284 | 54.323 | 46.432 | 65.842 | 1.00 | 42.46 | AAAA | N |
| ATOH | 2723 | H | GLY | 285 | 54.931 | 45.699 | 61.562 | 1.00 | 40.10 | AAAA | N |
| ATOH | 2725 | CA | GLY | 285 | 55.971 | 45.815 | 60.593 | 1.00 | 26.91 | AAAA | C |
| ATOH | 2726 | C | GLY | 285 | 56.091 | 44.468 | 59.848 | 1.00 | 33.12 | AAAA | C |
| ATOH | 2727 | O | GLY | 285 | 55.584 | 43.331 | 60.187 | 1.00 | 29.51 | AAAA | O |
| ATOH | 2729 | H | SER | 286 | 56.915 | 44.619 | 59.766 | 1.00 | 26.53 | AAAA | H |
| ATOH | 2730 | CA | SER | 286 | 57.109 | 43.395 | 57.975 | 1.00 | 32.67 | AAAA | C |
| ATOH | 2731 | CB | SER | 286 | 57.944 | 43.681 | 56.757 | 1.00 | 33.19 | AAAA | C |
| ATOH | 2732 | CG | SER | 286 | 58.283 | 42.480 | 56.014 | 1.00 | 31.95 | AAAA | O |
| ATOH | 2734 | C | SER | 286 | 57.750 | 42.310 | 58.836 | 1.00 | 34.57 | AAAA | C |
| ATOH | 2735 | O | SER | 286 | 56.700 | 42.495 | 59.607 | 1.00 | 44.29 | AAAA | O |
| ATOH | 2736 | H | GLN | 287 | 57.227 | 41.148 | 58.940 | 1.00 | 34.45 | AAAA | N |
| ATOH | 2738 | CA | GLN | 287 | 57.738 | 40.025 | 59.634 | 1.00 | 35.25 | AAAA | C |
| ATOH | 2739 | CB | GLN | 287 | 59.139 | 39.610 | 59.083 | 1.00 | 27.97 | AAAA | C |
| ATOH | 2740 | CG | GLN | 287 | 59.037 | 39.134 | 57.664 | 1.00 | 26.61 | AAAA | C |
| ATOH | 2741 | CD | GLN | 287 | 58.539 | 37.963 | 57.130 | 1.00 | 21.25 | AAAA | C |
| ATOH | 2742 | CE1 | GLN | 287 | 58.182 | 37.803 | 57.845 | 1.00 | 28.18 | AAAA | O |
| ATOH | 2743 | HE2 | GLN | 287 | 58.492 | 37.832 | 58.782 | 1.00 | 27.55 | AAAA | N |
| ATOH | 2746 | C | GLN | 287 | 57.773 | 40.295 | 61.111 | 1.00 | 30.25 | AAAA | C |
| ATOH | 2747 | O | GLN | 287 | 58.163 | 39.415 | 61.909 | 1.00 | 32.78 | AAAA | O |
| ATOH | 2748 | H | SER | 288 | 57.021 | 41.217 | 61.624 | 1.00 | 32.49 | AAAA | H |
| ATOH | 2750 | CA | SER | 288 | 56.696 | 41.322 | 63.043 | 1.00 | 28.98 | AAAA | C |
| ATOH | 2751 | CB | SER | 288 | 56.024 | 42.675 | 63.313 | 1.00 | 35.79 | AAAA | C |
| ATOH | 2752 | CG | SER | 288 | 55.639 | 42.612 | 64.701 | 1.00 | 36.61 | AAAA | O |
| ATOH | 2754 | C | SER | 288 | 55.665 | 40.285 | 63.442 | 1.00 | 28.96 | AAAA | C |
| ATOH | 2755 | O | SER | 288 | 54.993 | 39.776 | 62.553 | 1.00 | 31.16 | AAAA | O |
| ATOH | 2756 | H | MET | 289 | 55.774 | 39.720 | 64.621 | 1.00 | 32.51 | AAAA | H |
| ATOH | 2758 | CA | MET | 289 | 54.875 | 38.697 | 65.105 | 1.00 | 34.53 | AAAA | C |
| ATOH | 2759 | CB | MET | 289 | 55.507 | 37.823 | 66.153 | 1.00 | 30.31 | AAAA | C |
| ATOH | 2760 | CG | MET | 289 | 56.571 | 36.872 | 65.680 | 1.00 | 40.50 | AAAA | C |
| ATOH | 2761 | SD | MET | 289 | 56.977 | 35.623 | 66.881 | 1.00 | 31.65 | AAAA | S |
| ATOH | 2762 | CE | MET | 289 | 55.745 | 34.315 | 66.508 | 1.00 | 30.47 | AAAA | C |
| ATOH | 2763 | C | MET | 289 | 53.557 | 39.286 | 65.703 | 1.00 | 35.55 | AAAA | C |
| ATOH | 2764 | O | MET | 289 | 52.630 | 38.512 | 66.014 | 1.00 | 38.37 | AAAA | O |
| ATOH | 2765 | H | TYR | 290 | 53.380 | 40.565 | 65.742 | 1.00 | 29.54 | AAAA | H |
| ATOH | 2767 | CA | TYR | 290 | 52.363 | 41.358 | 66.297 | 1.00 | 38.81 | AAAA | C |
| ATOH | 2768 | CB | TYR | 290 | 52.947 | 42.589 | 67.042 | 1.00 | 36.72 | AAAA | C |
| ATOH | 2769 | CG | TYR | 290 | 53.570 | 42.184 | 68.351 | 1.00 | 41.94 | AAAA | C |
| ATOH | 2770 | CD1 | TYR | 290 | 54.932 | 41.780 | 68.350 | 1.00 | 37.79 | AAAA | C |
| ATOH | 2771 | CE1 | TYR | 290 | 55.548 | 41.369 | 69.503 | 1.00 | 32.60 | AAAA | C |
| ATOH | 2772 | CE2 | TYR | 290 | 52.887 | 42.157 | 69.570 | 1.00 | 39.93 | AAAA | C |
| ATOH | 2773 | CE2 | TYR | 290 | 53.501 | 41.750 | 70.748 | 1.00 | 36.16 | AAAA | C |
| ATOH | 2774 | CE | TYR | 290 | 54.822 | 41.355 | 70.693 | 1.00 | 38.85 | AAAA | C |
| ATOH | 2775 | OH | TYR | 290 | 55.581 | 40.923 | 71.751 | 1.00 | 43.41 | AAAA | O |
| ATOH | 2777 | C | TYR | 290 | 51.361 | 41.955 | 65.270 | 1.00 | 45.54 | AAAA | C |
| ATOH | 2778 | O | TYR | 290 | 51.733 | 42.520 | 64.227 | 1.00 | 47.10 | AAAA | O |
| ATOH | 2779 | H | CYS | 291 | 50.071 | 41.699 | 65.537 | 1.00 | 44.68 | AAAA | H |
| ATOH | 2781 | CA | CYS | 291 | 49.017 | 42.205 | 64.695 | 1.00 | 47.20 | AAAA | C |
| ATOH | 2782 | C | CYS | 291 | 48.295 | 43.434 | 65.194 | 1.00 | 46.06 | AAAA | C |
| ATOH | 2783 | O | CYS | 291 | 47.892 | 43.550 | 66.343 | 1.00 | 49.45 | AAAA | O |
| ATOH | 2784 | CB | CYS | 291 | 47.973 | 41.103 | 64.483 | 1.00 | 43.44 | AAAA | C |
| ATOH | 2785 | SG | CYS | 291 | 48.766 | 39.715 | 63.683 | 1.00 | 45.49 | AAAA | S |
| ATOH | 2786 | H | ILE | 292 | 48.136 | 44.453 | 64.365 | 1.00 | 46.82 | AAAA | H |
| ATOH | 2788 | CA | ILE | 292 | 47.399 | 45.651 | 64.755 | 1.00 | 50.64 | AAAA | C |
| ATOH | 2789 | CB | ILE | 292 | 48.267 | 46.932 | 64.779 | 1.00 | 39.19 | AAAA | C |
| ATOH | 2790 | CG2 | ILE | 292 | 49.291 | 46.885 | 65.861 | 1.00 | 44.39 | AAAA | C |
| ATOH | 2791 | CG1 | ILE | 292 | 48.920 | 47.095 | 63.402 | 1.00 | 44.25 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 2790 | CD | ILE | 292 | 49.234 | 48.568 | 63.108 | 1.00 | 32.80 | AAAA | C |
| ATOH | 2793 | C | ILE | 292 | 46.240 | 46.003 | 63.806 | 1.00 | 50.01 | AAAA | C |
| ATOH | 2794 | O | ILE | 292 | 46.165 | 45.526 | 62.670 | 1.00 | 46.64 | AAAA | O |
| ATOH | 2795 | H | PRO | 293 | 45.150 | 46.507 | 64.385 | 1.00 | 51.86 | AAAA | H |
| ATOH | 2796 | CD | PRO | 293 | 45.009 | 46.804 | 65.839 | 1.00 | 51.05 | AAAA | C |
| ATOH | 2797 | CA | PRO | 293 | 43.958 | 46.930 | 63.675 | 1.00 | 51.40 | AAAA | C |
| ATOH | 2798 | CB | PRO | 293 | 43.170 | 47.784 | 64.681 | 1.00 | 49.00 | AAAA | C |
| ATOH | 2799 | CG | PRO | 293 | 43.533 | 47.112 | 65.951 | 1.00 | 53.73 | AAAA | C |
| ATOH | 2800 | C | PRO | 293 | 44.253 | 47.870 | 62.525 | 1.00 | 51.68 | AAAA | C |
| ATOH | 2801 | O | PRO | 293 | 45.053 | 48.788 | 62.737 | 1.00 | 51.92 | AAAA | O |
| ATOH | 2802 | H | CYS | 294 | 43.607 | 47.621 | 61.408 | 1.00 | 50.66 | AAAA | H |
| ATOH | 2804 | CA | CYS | 294 | 43.811 | 48.464 | 60.254 | 1.00 | 57.90 | AAAA | C |
| ATOH | 2805 | C | CYS | 294 | 43.219 | 49.848 | 60.345 | 1.00 | 59.59 | AAAA | C |
| ATOH | 2806 | O | CYS | 294 | 43.744 | 50.814 | 59.785 | 1.00 | 60.87 | AAAA | O |
| ATOH | 2807 | CB | CYS | 294 | 43.229 | 47.686 | 59.046 | 1.00 | 57.59 | AAAA | C |
| ATOH | 2808 | SG | CYS | 294 | 44.408 | 46.460 | 58.563 | 1.00 | 51.12 | AAAA | S |
| ATOH | 2809 | H | ALA | 295 | 42.009 | 50.031 | 60.854 | 1.00 | 65.87 | AAAA | H |
| ATOH | 2811 | CA | ALA | 295 | 41.391 | 51.386 | 60.804 | 1.00 | 71.19 | AAAA | C |
| ATOH | 2812 | CB | ALA | 295 | 42.311 | 52.459 | 61.393 | 1.00 | 63.82 | AAAA | C |
| ATOH | 2813 | C | ALA | 295 | 40.971 | 51.770 | 59.370 | 1.00 | 69.17 | AAAA | C |
| ATOH | 2814 | O | ALA | 295 | 41.421 | 52.717 | 58.762 | 1.00 | 64.70 | AAAA | O |
| ATOH | 2815 | H | GLY | 296 | 40.153 | 50.920 | 58.775 | 1.00 | 71.30 | AAAA | H |
| ATOH | 2817 | CA | GLY | 296 | 39.640 | 51.049 | 57.416 | 1.00 | 72.66 | AAAA | C |
| ATOH | 2818 | C | GLY | 296 | 39.895 | 49.686 | 56.769 | 1.00 | 74.20 | AAAA | C |
| ATOH | 2819 | O | GLY | 296 | 40.408 | 48.819 | 57.490 | 1.00 | 75.04 | AAAA | O |
| ATOH | 2820 | H | PRO | 297 | 39.561 | 49.540 | 55.497 | 1.00 | 71.88 | AAAA | H |
| ATOH | 2821 | CD | PRO | 297 | 38.928 | 50.561 | 54.637 | 1.00 | 72.15 | AAAA | C |
| ATOH | 2822 | CA | PRO | 297 | 39.958 | 48.344 | 54.777 | 1.00 | 68.23 | AAAA | C |
| ATOH | 2823 | CB | PRO | 297 | 39.488 | 48.603 | 53.369 | 1.00 | 72.57 | AAAA | C |
| ATOH | 2824 | CG | PRO | 297 | 38.470 | 49.687 | 53.490 | 1.00 | 74.04 | AAAA | C |
| ATOH | 2825 | C | PRO | 297 | 41.480 | 48.306 | 54.860 | 1.00 | 65.78 | AAAA | C |
| ATOH | 2826 | O | PRO | 297 | 42.147 | 49.323 | 54.997 | 1.00 | 62.72 | AAAA | O |
| ATOH | 2827 | H | CYS | 298 | 42.039 | 47.135 | 55.073 | 1.00 | 63.85 | AAAA | H |
| ATOH | 2829 | CA | CYS | 298 | 43.464 | 46.953 | 55.248 | 1.00 | 54.47 | AAAA | C |
| ATOH | 2830 | C | CYS | 298 | 44.109 | 47.303 | 53.908 | 1.00 | 54.56 | AAAA | C |
| ATOH | 2831 | O | CYS | 298 | 43.621 | 47.030 | 52.820 | 1.00 | 54.83 | AAAA | O |
| ATOH | 2832 | CB | CYS | 298 | 43.665 | 46.544 | 55.669 | 1.00 | 47.65 | AAAA | C |
| ATOH | 2833 | SG | CYS | 298 | 43.501 | 46.115 | 57.371 | 1.00 | 46.12 | AAAA | S |
| ATOH | 2834 | H | PRO | 299 | 45.310 | 47.876 | 53.967 | 1.00 | 49.83 | AAAA | H |
| ATOH | 2835 | CD | PRO | 299 | 46.087 | 49.168 | 55.194 | 1.00 | 48.14 | AAAA | C |
| ATOH | 2836 | CA | PRO | 299 | 46.055 | 48.212 | 52.787 | 1.00 | 43.67 | AAAA | C |
| ATOH | 2837 | CB | PRO | 299 | 47.267 | 49.965 | 53.281 | 1.00 | 44.08 | AAAA | C |
| ATOH | 2838 | CG | PRO | 299 | 47.454 | 49.361 | 54.628 | 1.00 | 51.38 | AAAA | C |
| ATOH | 2839 | C | PRO | 299 | 46.341 | 46.969 | 52.010 | 1.00 | 38.86 | AAAA | C |
| ATOH | 2840 | O | PRO | 299 | 46.372 | 46.874 | 52.546 | 1.00 | 42.25 | AAAA | O |
| ATOH | 2841 | H | LYS | 300 | 46.310 | 47.073 | 50.712 | 1.00 | 38.30 | AAAA | H |
| ATOH | 2843 | CA | LYS | 300 | 46.484 | 46.959 | 49.812 | 1.00 | 42.62 | AAAA | C |
| ATOH | 2844 | CB | LYS | 300 | 45.176 | 46.226 | 49.595 | 1.00 | 34.28 | AAAA | C |
| ATOH | 2845 | CG | LYS | 300 | 45.346 | 43.901 | 48.920 | 1.00 | 41.45 | AAAA | C |
| ATOH | 2846 | CD | LYS | 300 | 44.013 | 45.413 | 48.378 | 1.00 | 49.31 | AAAA | C |
| ATOH | 2847 | CE | LYS | 300 | 44.388 | 42.027 | 47.787 | 1.00 | 48.57 | AAAA | C |
| ATOH | 2848 | HD | LYS | 300 | 43.662 | 42.031 | 46.478 | 1.00 | 63.70 | AAAA | H |
| ATOH | 2852 | C | LYS | 300 | 46.964 | 46.479 | 49.432 | 1.00 | 48.72 | AAAA | C |
| ATOH | 2853 | O | LYS | 300 | 46.413 | 47.393 | 47.776 | 1.00 | 46.09 | AAAA | O |
| ATOH | 2854 | H | VAL | 301 | 48.150 | 45.994 | 48.054 | 1.00 | 48.15 | AAAA | H |
| ATOH | 2856 | CA | VAL | 301 | 48.802 | 46.462 | 46.871 | 1.00 | 44.52 | AAAA | C |
| ATOH | 2857 | CB | VAL | 301 | 50.292 | 46.729 | 47.074 | 1.00 | 51.52 | AAAA | C |
| ATOH | 2858 | CG1 | VAL | 301 | 51.008 | 47.200 | 45.796 | 1.00 | 43.07 | AAAA | C |
| ATOH | 2859 | CG2 | VAL | 301 | 50.495 | 47.794 | 48.141 | 1.00 | 49.50 | AAAA | C |
| ATOH | 2860 | C | VAL | 301 | 48.526 | 45.410 | 45.837 | 1.00 | 44.59 | AAAA | C |
| ATOH | 2861 | O | VAL | 301 | 48.913 | 44.291 | 46.060 | 1.00 | 43.70 | AAAA | O |
| ATOH | 2862 | H | CYS | 302 | 47.910 | 45.816 | 44.718 | 1.00 | 47.98 | AAAA | H |
| ATOH | 2864 | CA | CYS | 302 | 47.645 | 44.735 | 43.739 | 1.00 | 55.19 | AAAA | C |
| ATOH | 2865 | C | CYS | 302 | 48.594 | 44.968 | 42.583 | 1.00 | 57.64 | AAAA | C |
| ATOH | 2866 | O | CYS | 302 | 48.852 | 46.152 | 42.343 | 1.00 | 60.23 | AAAA | O |
| ATOH | 2867 | CB | CYS | 302 | 46.186 | 44.630 | 43.330 | 1.00 | 68.30 | AAAA | C |
| ATOH | 2868 | SG | CYS | 302 | 45.070 | 44.360 | 44.751 | 1.00 | 70.31 | AAAA | S |
| ATOH | 2869 | H | GLU | 303 | 49.183 | 43.921 | 42.075 | 1.00 | 58.15 | AAAA | H |
| ATOH | 2871 | CA | GLU | 303 | 50.174 | 43.932 | 41.034 | 1.00 | 62.85 | AAAA | C |
| ATOH | 2872 | CB | GLU | 303 | 51.603 | 44.006 | 41.595 | 1.00 | 67.85 | AAAA | C |
| ATOH | 2873 | CG | GLU | 303 | 51.760 | 43.487 | 43.014 | 0.01 | 67.46 | AAAA | C |
| ATOH | 2874 | CD | GLU | 303 | 51.989 | 41.992 | 43.097 | 0.01 | 67.94 | AAAA | C |
| ATOH | 2875 | OE1 | GLU | 303 | 53.011 | 41.514 | 42.561 | 0.01 | 67.67 | AAAA | O |
| ATOH | 2876 | OE2 | GLU | 303 | 51.147 | 41.290 | 43.697 | 0.01 | 67.65 | AAAA | O |
| ATOH | 2877 | C | GLU | 303 | 50.096 | 42.662 | 40.194 | 1.00 | 64.12 | AAAA | C |
| ATOH | 2878 | O | GLU | 303 | 50.162 | 41.562 | 40.708 | 1.00 | 65.08 | AAAA | O |
| ATOH | 2879 | N | GLU | 304 | 49.867 | 42.794 | 38.904 | 1.00 | 67.37 | AAAA | H |
| ATOH | 2881 | CA | GLU | 304 | 49.672 | 41.583 | 38.094 | 1.00 | 74.63 | AAAA | C |
| ATOH | 2882 | CB | GLU | 304 | 48.285 | 41.596 | 37.458 | 1.00 | 71.71 | AAAA | C |
| ATOH | 2883 | CG | GLU | 304 | 47.339 | 42.663 | 38.031 | 1.00 | 84.54 | AAAA | C |
| ATOH | 2884 | CD | GLU | 304 | 45.930 | 42.152 | 39.185 | 1.00 | 87.56 | AAAA | C |
| ATOH | 2885 | OE1 | GLU | 304 | 45.438 | 41.571 | 37.179 | 1.00 | 89.13 | AAAA | O |
| ATOH | 2886 | OE2 | GLU | 304 | 45.249 | 42.269 | 39.233 | 1.00 | 93.19 | AAAA | O |
| ATOH | 2887 | C | GLU | 304 | 50.866 | 41.307 | 37.190 | 1.00 | 76.10 | AAAA | C |
| ATOH | 2888 | O | GLU | 304 | 51.911 | 41.962 | 37.217 | 1.00 | 74.78 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 2889 | H | GLU | 305 | 50.899 | 40.126 | 36.568 | 1.00 | 77.31 | AAAA | H |
| ATOH | 2891 | CA | GLU | 305 | 51.932 | 39.656 | 35.674 | 1.00 | 75.90 | AAAA | C |
| ATOH | 2892 | CB | GLU | 305 | 51.467 | 38.380 | 34.970 | 1.00 | 79.95 | AAAA | C |
| ATOH | 2893 | CG | GLU | 305 | 52.307 | 37.937 | 33.807 | 1.00 | 87.28 | AAAA | C |
| ATOH | 2894 | CD | GLU | 305 | 51.758 | 36.891 | 32.886 | 0.01 | 83.39 | AAAA | C |
| ATOH | 2895 | OE1 | GLU | 305 | 50.762 | 36.234 | 33.252 | 0.01 | 83.66 | AAAA | O |
| ATOH | 2896 | OE2 | GLU | 305 | 52.310 | 36.700 | 31.780 | 0.01 | 83.73 | AAAA | O |
| ATOH | 2897 | C | GLU | 305 | 52.276 | 40.737 | 34.666 | 1.00 | 75.97 | AAAA | C |
| ATOH | 2898 | O | GLU | 305 | 53.381 | 41.268 | 34.613 | 1.00 | 76.54 | AAAA | O |
| ATOH | 2899 | H | LYS | 306 | 51.291 | 41.181 | 33.888 | 1.00 | 78.22 | AAAA | H |
| ATOH | 2901 | CA | LYS | 306 | 51.479 | 42.328 | 33.004 | 1.00 | 75.99 | AAAA | C |
| ATOH | 2902 | CB | LYS | 306 | 50.467 | 42.253 | 31.855 | 1.00 | 79.78 | AAAA | C |
| ATOH | 2903 | CG | LYS | 306 | 51.208 | 42.227 | 30.527 | 1.00 | 94.52 | AAAA | C |
| ATOH | 2904 | CD | LYS | 306 | 50.313 | 42.191 | 29.314 | 1.00 | 92.78 | AAAA | C |
| ATOH | 2905 | CE | LYS | 306 | 50.740 | 43.227 | 28.261 | 1.00 | 97.10 | AAAA | C |
| ATOH | 2906 | HE | LYS | 306 | 50.938 | 44.554 | 28.929 | 1.00 | 84.87 | AAAA | H |
| ATOH | 2910 | C | LYS | 306 | 51.381 | 43.669 | 33.703 | 1.00 | 73.85 | AAAA | C |
| ATOH | 2911 | O | LYS | 306 | 50.703 | 43.862 | 34.718 | 1.00 | 76.08 | AAAA | O |
| ATOH | 2912 | H | LYS | 307 | 52.000 | 44.700 | 33.180 | 1.00 | 71.15 | AAAA | H |
| ATOH | 2914 | CA | LYS | 307 | 51.934 | 46.053 | 33.692 | 1.00 | 69.45 | AAAA | C |
| ATOH | 2915 | CB | LYS | 307 | 53.022 | 46.903 | 33.008 | 1.00 | 79.64 | AAAA | C |
| ATOH | 2916 | CG | LYS | 307 | 54.419 | 46.837 | 33.564 | 1.00 | 78.88 | AAAA | C |
| ATOH | 2917 | CD | LYS | 307 | 55.257 | 48.084 | 33.374 | 1.00 | 85.84 | AAAA | C |
| ATOH | 2918 | CE | LYS | 307 | 55.708 | 48.215 | 31.924 | 1.00 | 97.07 | AAAA | C |
| ATOH | 2919 | HE | LYS | 307 | 54.649 | 48.840 | 31.067 | 1.00 | 97.80 | AAAA | H |
| ATOH | 2923 | C | LYS | 307 | 50.562 | 46.716 | 33.525 | 1.00 | 67.97 | AAAA | C |
| ATOH | 2924 | O | LYS | 307 | 50.010 | 47.369 | 34.431 | 1.00 | 64.46 | AAAA | O |
| ATOH | 2925 | H | THR | 308 | 49.979 | 46.661 | 32.323 | 1.00 | 65.84 | AAAA | H |
| ATOH | 2927 | CA | THR | 308 | 48.709 | 47.319 | 32.091 | 1.00 | 64.56 | AAAA | C |
| ATOH | 2928 | CB | THR | 308 | 48.714 | 47.977 | 30.711 | 1.00 | 59.91 | AAAA | C |
| ATOH | 2929 | CG1 | THR | 308 | 49.834 | 48.843 | 30.577 | 1.00 | 61.97 | AAAA | O |
| ATOH | 2931 | CG2 | THR | 308 | 47.392 | 48.742 | 30.561 | 1.00 | 63.64 | AAAA | C |
| ATOH | 2932 | C | THR | 308 | 47.514 | 46.379 | 32.234 | 1.00 | 61.82 | AAAA | C |
| ATOH | 2933 | O | THR | 308 | 47.412 | 45.415 | 31.477 | 1.00 | 62.05 | AAAA | O |
| ATOH | 2934 | H | LYS | 309 | 46.675 | 46.719 | 33.211 | 1.00 | 55.66 | AAAA | H |
| ATOH | 2936 | CA | LYS | 309 | 45.456 | 45.926 | 33.445 | 1.00 | 54.67 | AAAA | C |
| ATOH | 2937 | CB | LYS | 309 | 45.043 | 45.880 | 34.904 | 1.00 | 56.82 | AAAA | C |
| ATOH | 2939 | CG | LYS | 309 | 43.601 | 45.541 | 35.223 | 1.00 | 57.50 | AAAA | C |
| ATOH | 2939 | CD | LYS | 309 | 43.390 | 44.039 | 35.086 | 1.00 | 59.50 | AAAA | C |
| ATOH | 2940 | CE | LYS | 309 | 42.703 | 43.448 | 36.324 | 1.00 | 57.31 | AAAA | C |
| ATOH | 2941 | HE | LYS | 309 | 42.758 | 41.954 | 36.236 | 1.00 | 57.22 | AAAA | H |
| ATOH | 2945 | C | LYS | 309 | 44.391 | 46.570 | 32.549 | 1.00 | 51.21 | AAAA | C |
| ATOH | 2946 | O | LYS | 309 | 44.074 | 47.763 | 32.680 | 1.00 | 47.23 | AAAA | O |
| ATOH | 2947 | H | THR | 310 | 43.895 | 45.772 | 31.610 | 1.00 | 47.67 | AAAA | H |
| ATOH | 2949 | CA | THR | 310 | 42.862 | 45.329 | 30.733 | 1.00 | 51.89 | AAAA | C |
| ATOH | 2950 | CB | THR | 310 | 43.161 | 46.015 | 29.266 | 1.00 | 54.81 | AAAA | C |
| ATOH | 2951 | CG1 | THR | 310 | 41.909 | 45.710 | 28.635 | 1.00 | 66.29 | AAAA | C |
| ATOH | 2953 | CG2 | THR | 310 | 44.032 | 44.791 | 29.139 | 1.00 | 55.19 | AAAA | C |
| ATOH | 2954 | C | THR | 310 | 41.468 | 45.941 | 31.117 | 1.00 | 51.15 | AAAA | C |
| ATOH | 2956 | O | THR | 310 | 41.162 | 44.680 | 30.991 | 1.00 | 49.27 | AAAA | O |
| ATOH | 2956 | H | ILE | 311 | 40.684 | 46.706 | 31.732 | 1.00 | 50.18 | AAAA | H |
| ATOH | 2958 | CA | ILE | 311 | 39.363 | 46.453 | 32.276 | 1.00 | 48.67 | AAAA | C |
| ATOH | 2959 | CB | ILE | 311 | 39.120 | 47.396 | 33.462 | 1.00 | 49.27 | AAAA | C |
| ATOH | 2960 | CG2 | ILE | 311 | 37.655 | 47.596 | 33.799 | 1.00 | 50.72 | AAAA | C |
| ATOH | 2961 | CG1 | ILE | 311 | 39.896 | 46.930 | 34.699 | 1.00 | 41.34 | AAAA | C |
| ATOH | 2962 | CD1 | ILE | 311 | 39.847 | 48.073 | 35.739 | 1.00 | 52.22 | AAAA | C |
| ATOH | 2963 | C | ILE | 311 | 38.334 | 46.729 | 31.186 | 1.00 | 45.37 | AAAA | C |
| ATOH | 2964 | O | ILE | 311 | 38.132 | 47.875 | 30.758 | 1.00 | 37.14 | AAAA | O |
| ATOH | 2965 | H | ASP | 312 | 37.871 | 45.678 | 30.524 | 1.00 | 50.10 | AAAA | H |
| ATOH | 2967 | CA | ASP | 312 | 36.991 | 45.842 | 29.377 | 1.00 | 56.35 | AAAA | C |
| ATOH | 2968 | CB | ASP | 312 | 37.546 | 45.152 | 28.128 | 1.00 | 59.45 | AAAA | C |
| ATOH | 2969 | CG | ASP | 312 | 37.761 | 43.671 | 28.382 | 1.00 | 65.64 | AAAA | C |
| ATOH | 2970 | OD1 | ASP | 312 | 38.525 | 43.034 | 27.636 | 1.00 | 72.60 | AAAA | O |
| ATOH | 2971 | OD2 | ASP | 312 | 37.154 | 43.176 | 29.349 | 1.00 | 66.86 | AAAA | O |
| ATOH | 2972 | C | ASP | 312 | 35.589 | 45.337 | 29.693 | 1.00 | 59.39 | AAAA | C |
| ATOH | 2973 | O | ASP | 312 | 34.729 | 45.007 | 28.867 | 1.00 | 61.00 | AAAA | O |
| ATOH | 2974 | H | SER | 313 | 35.278 | 45.290 | 30.976 | 1.00 | 61.17 | AAAA | H |
| ATOH | 2976 | CA | SER | 313 | 34.053 | 44.683 | 31.459 | 1.00 | 55.73 | AAAA | C |
| ATOH | 2977 | CB | SER | 313 | 34.121 | 43.201 | 31.083 | 1.00 | 48.22 | AAAA | C |
| ATOH | 2978 | CG | SER | 313 | 34.373 | 42.514 | 32.282 | 1.00 | 57.89 | AAAA | O |
| ATOH | 2980 | C | SER | 313 | 33.998 | 44.818 | 32.941 | 1.00 | 57.87 | AAAA | C |
| ATOH | 2981 | O | SER | 313 | 34.802 | 45.506 | 33.537 | 1.00 | 66.47 | AAAA | O |
| ATOH | 2982 | H | VAL | 314 | 33.001 | 44.205 | 33.545 | 1.00 | 64.35 | AAAA | H |
| ATOH | 2984 | CA | VAL | 314 | 32.949 | 44.305 | 35.016 | 1.00 | 64.39 | AAAA | C |
| ATOH | 2985 | CB | VAL | 314 | 31.360 | 44.340 | 35.343 | 1.00 | 69.57 | AAAA | C |
| ATOH | 2986 | CG1 | VAL | 314 | 31.024 | 43.693 | 36.681 | 1.00 | 65.60 | AAAA | C |
| ATOH | 2987 | CG2 | VAL | 314 | 30.927 | 45.823 | 35.319 | 1.00 | 65.27 | AAAA | C |
| ATOH | 2988 | C | VAL | 314 | 33.492 | 43.088 | 35.638 | 1.00 | 62.65 | AAAA | C |
| ATOH | 2989 | O | VAL | 314 | 34.029 | 43.141 | 36.704 | 1.00 | 63.92 | AAAA | O |
| ATOH | 2990 | H | THR | 315 | 33.468 | 42.011 | 34.878 | 1.00 | 61.82 | AAAA | H |
| ATOH | 2992 | CA | THR | 315 | 34.029 | 40.752 | 35.284 | 1.00 | 63.44 | AAAA | C |
| ATOH | 2993 | CB | THR | 315 | 33.618 | 39.628 | 34.314 | 1.00 | 65.54 | AAAA | C |
| ATOH | 2994 | CG1 | THR | 315 | 32.403 | 40.004 | 33.634 | 1.00 | 74.05 | AAAA | O |
| ATOH | 2996 | CG2 | THR | 315 | 33.339 | 38.366 | 35.104 | 1.00 | 64.86 | AAAA | C |
| ATOH | 2997 | C | THR | 315 | 35.541 | 40.871 | 35.323 | 1.00 | 65.62 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|--------|------|---|
| ATOH | 2998 | O | THR | 315 | 36.217 | 40.339 | 36.206 | 1.00 | 66.41 | AAAA | O |
| ATOH | 2999 | H | SER | 316 | 36.071 | 41.593 | 34.332 | 1.00 | 63.28 | AAAA | H |
| ATOH | 3001 | CA | SER | 316 | 37.500 | 41.793 | 34.215 | 1.00 | 58.72 | AAAA | C |
| ATOH | 3002 | CB | SER | 316 | 37.785 | 42.537 | 32.900 | 1.00 | 52.20 | AAAA | C |
| ATOH | 3003 | OG | SER | 316 | 37.298 | 43.859 | 32.933 | 1.00 | 48.04 | AAAA | O |
| ATOH | 3005 | C | SER | 316 | 38.077 | 42.573 | 35.387 | 1.00 | 58.91 | AAAA | C |
| ATOH | 3006 | O | SER | 316 | 39.293 | 42.522 | 35.520 | 1.00 | 59.86 | AAAA | O |
| ATOH | 3007 | H | ALA | 317 | 37.310 | 43.362 | 36.111 | 1.00 | 55.86 | AAAA | H |
| ATOH | 3009 | CA | ALA | 317 | 37.750 | 44.184 | 37.191 | 1.00 | 57.17 | AAAA | C |
| ATOH | 3010 | CB | ALA | 317 | 36.833 | 45.409 | 37.269 | 1.00 | 54.23 | AAAA | C |
| ATOH | 3011 | C | ALA | 317 | 37.689 | 43.487 | 38.538 | 1.00 | 62.05 | AAAA | C |
| ATOH | 3012 | O | ALA | 317 | 37.702 | 44.128 | 39.599 | 1.00 | 60.30 | AAAA | O |
| ATOH | 3013 | H | GLN | 318 | 37.361 | 42.205 | 38.523 | 1.00 | 67.91 | AAAA | H |
| ATOH | 3015 | CA | GLN | 318 | 37.185 | 41.380 | 39.713 | 1.00 | 70.72 | AAAA | C |
| ATOH | 3016 | CB | GLN | 318 | 36.857 | 39.956 | 39.293 | 1.00 | 74.48 | AAAA | C |
| ATOH | 3017 | CG | GLN | 318 | 36.624 | 38.947 | 40.383 | 1.00 | 89.82 | AAAA | C |
| ATOH | 3018 | CD | GLN | 318 | 35.265 | 39.080 | 41.048 | 1.00 | 92.69 | AAAA | C |
| ATOH | 3019 | OE1 | GLN | 318 | 34.256 | 39.807 | 40.391 | 1.00 | 98.57 | AAAA | O |
| ATOH | 3020 | HE2 | GLN | 318 | 35.356 | 39.509 | 42.308 | 1.00 | 92.51 | AAAA | N |
| ATOH | 3023 | C | GLN | 318 | 38.380 | 41.413 | 40.653 | 1.00 | 72.63 | AAAA | C |
| ATOH | 3024 | O | GLN | 318 | 38.294 | 41.855 | 41.804 | 1.00 | 68.92 | AAAA | O |
| ATOH | 3025 | H | NET | 319 | 39.562 | 41.062 | 40.153 | 1.00 | 75.18 | AAAA | H |
| ATOH | 3027 | CA | NET | 319 | 40.846 | 41.175 | 40.826 | 1.00 | 71.85 | AAAA | C |
| ATOH | 3028 | CB | NET | 319 | 41.950 | 40.960 | 39.772 | 1.00 | 82.00 | AAAA | C |
| ATOH | 3029 | CG | NET | 319 | 41.740 | 39.644 | 39.050 | 1.00 | 91.16 | AAAA | C |
| ATOH | 3030 | SD | NET | 319 | 43.123 | 38.482 | 39.185 | 1.00 | 106.72 | AAAA | S |
| ATOH | 3031 | CE | NET | 319 | 42.486 | 37.105 | 38.231 | 1.00 | 97.56 | AAAA | C |
| ATOH | 3032 | C | NET | 319 | 41.118 | 42.509 | 41.471 | 1.00 | 67.68 | AAAA | C |
| ATOH | 3033 | O | NET | 319 | 41.597 | 42.541 | 42.612 | 1.00 | 69.73 | AAAA | O |
| ATOH | 3034 | H | LEU | 320 | 40.740 | 43.639 | 40.887 | 1.00 | 62.95 | AAAA | H |
| ATOH | 3036 | CA | LEU | 320 | 40.907 | 44.938 | 41.531 | 1.00 | 62.31 | AAAA | C |
| ATOH | 3037 | CB | LEU | 320 | 40.440 | 46.085 | 40.623 | 1.00 | 54.93 | AAAA | C |
| ATOH | 3038 | CG | LEU | 320 | 41.091 | 46.163 | 39.238 | 1.00 | 53.48 | AAAA | C |
| ATOH | 3039 | CD1 | LEU | 320 | 41.005 | 47.552 | 38.692 | 1.00 | 51.31 | AAAA | C |
| ATOH | 3040 | CD2 | LEU | 320 | 42.557 | 45.709 | 39.403 | 1.00 | 58.43 | AAAA | C |
| ATOH | 3041 | C | LEU | 320 | 40.209 | 45.008 | 42.881 | 1.00 | 60.30 | AAAA | C |
| ATOH | 3042 | O | LEU | 320 | 40.344 | 45.969 | 43.661 | 1.00 | 58.72 | AAAA | O |
| ATOH | 3043 | H | GLN | 321 | 39.267 | 44.106 | 43.112 | 1.00 | 59.62 | AAAA | H |
| ATOH | 3046 | CA | GLN | 321 | 38.482 | 44.128 | 44.343 | 1.00 | 63.50 | AAAA | C |
| ATOH | 3046 | CB | GLN | 321 | 37.373 | 43.289 | 44.250 | 1.00 | 62.52 | AAAA | C |
| ATOH | 3047 | CG | GLN | 321 | 36.611 | 42.884 | 45.522 | 1.00 | 56.83 | AAAA | C |
| ATOH | 3048 | CD | GLN | 321 | 35.337 | 42.064 | 45.291 | 1.00 | 68.77 | AAAA | C |
| ATOH | 3049 | OE1 | GLN | 321 | 35.360 | 40.969 | 44.718 | 1.00 | 70.37 | AAAA | O |
| ATOH | 3050 | HE2 | GLN | 321 | 34.218 | 40.632 | 45.764 | 1.00 | 63.77 | AAAA | N |
| ATOH | 3053 | C | GLN | 321 | 39.367 | 44.030 | 45.594 | 1.00 | 60.97 | AAAA | C |
| ATOH | 3054 | O | GLN | 321 | 40.262 | 43.196 | 45.782 | 1.00 | 57.29 | AAAA | O |
| ATOH | 3055 | H | GLY | 322 | 39.092 | 44.908 | 46.546 | 1.00 | 57.62 | AAAA | H |
| ATOH | 3057 | CA | GLY | 322 | 39.855 | 44.908 | 47.790 | 1.00 | 60.63 | AAAA | C |
| ATOH | 3058 | C | GLY | 322 | 41.126 | 45.773 | 47.812 | 1.00 | 61.79 | AAAA | C |
| ATOH | 3059 | O | GLY | 322 | 41.584 | 46.198 | 48.989 | 1.00 | 60.16 | AAAA | O |
| ATOH | 3060 | H | CYS | 323 | 41.719 | 46.124 | 46.676 | 1.00 | 60.03 | AAAA | H |
| ATOH | 3060 | CA | CYS | 323 | 42.938 | 46.845 | 46.528 | 1.00 | 54.20 | AAAA | C |
| ATOH | 3063 | C | CYS | 323 | 42.924 | 49.307 | 46.910 | 1.00 | 53.48 | AAAA | C |
| ATOH | 3064 | O | CYS | 323 | 42.105 | 49.148 | 46.503 | 1.00 | 56.43 | AAAA | O |
| ATOH | 3065 | CB | CYS | 323 | 43.458 | 46.822 | 45.086 | 1.00 | 53.33 | AAAA | C |
| ATOH | 3066 | SG | CYS | 323 | 43.325 | 45.222 | 44.248 | 1.00 | 66.22 | AAAA | S |
| ATOH | 3067 | H | THR | 324 | 43.994 | 48.718 | 47.580 | 1.00 | 49.83 | AAAA | H |
| ATOH | 3069 | CA | THR | 324 | 44.164 | 50.161 | 47.811 | 1.00 | 52.29 | AAAA | C |
| ATOH | 3070 | CB | THR | 324 | 44.623 | 50.324 | 49.264 | 1.00 | 52.84 | AAAA | C |
| ATOH | 3071 | CG1 | THR | 324 | 45.245 | 49.087 | 49.634 | 1.00 | 59.92 | AAAA | O |
| ATOH | 3073 | CG2 | THR | 324 | 43.432 | 50.517 | 50.193 | 1.00 | 60.00 | AAAA | C |
| ATOH | 3074 | C | THR | 324 | 45.154 | 50.802 | 46.844 | 1.00 | 48.91 | AAAA | C |
| ATOH | 3075 | O | THR | 324 | 45.277 | 52.016 | 46.710 | 1.00 | 46.90 | AAAA | O |
| ATOH | 3076 | H | ILE | 325 | 46.021 | 49.963 | 46.254 | 1.00 | 46.87 | AAAA | N |
| ATOH | 3078 | CA | ILE | 325 | 47.114 | 50.511 | 45.445 | 1.00 | 45.10 | AAAA | C |
| ATOH | 3079 | CB | ILE | 325 | 48.473 | 50.577 | 46.183 | 1.00 | 43.60 | AAAA | C |
| ATOH | 3080 | CG2 | ILE | 325 | 49.586 | 50.905 | 45.163 | 1.00 | 47.47 | AAAA | C |
| ATOH | 3081 | CG1 | ILE | 325 | 48.394 | 51.623 | 47.294 | 1.00 | 34.03 | AAAA | C |
| ATOH | 3082 | CD1 | ILE | 325 | 49.595 | 52.010 | 48.028 | 1.00 | 41.94 | AAAA | C |
| ATOH | 3083 | C | ILE | 325 | 47.265 | 49.642 | 44.229 | 1.00 | 42.89 | AAAA | C |
| ATOH | 3084 | O | ILE | 325 | 47.406 | 48.429 | 44.469 | 1.00 | 42.99 | AAAA | O |
| ATOH | 3085 | H | PHE | 326 | 47.170 | 50.238 | 43.042 | 1.00 | 41.19 | AAAA | H |
| ATOH | 3087 | CA | PHE | 326 | 47.312 | 49.334 | 41.880 | 1.00 | 42.89 | AAAA | C |
| ATOH | 3088 | CB | PHE | 326 | 46.166 | 49.437 | 40.877 | 1.00 | 39.15 | AAAA | C |
| ATOH | 3089 | CG | PHE | 326 | 46.403 | 48.474 | 39.738 | 1.00 | 38.03 | AAAA | C |
| ATOH | 3090 | CD1 | PHE | 326 | 46.186 | 47.125 | 39.951 | 1.00 | 39.68 | AAAA | C |
| ATOH | 3091 | CD2 | PHE | 326 | 46.917 | 48.892 | 38.525 | 1.00 | 37.31 | AAAA | C |
| ATOH | 3092 | CE1 | PHE | 326 | 46.447 | 46.139 | 39.023 | 1.00 | 36.52 | AAAA | C |
| ATOH | 3093 | CE2 | PHE | 326 | 47.136 | 47.919 | 37.551 | 1.00 | 45.74 | AAAA | C |
| ATOH | 3094 | CG | PHE | 326 | 46.924 | 46.570 | 37.787 | 1.00 | 39.92 | AAAA | C |
| ATOH | 3095 | C | PHE | 326 | 48.682 | 49.673 | 41.280 | 1.00 | 48.78 | AAAA | C |
| ATOH | 3096 | O | PHE | 326 | 49.024 | 50.826 | 40.966 | 1.00 | 51.39 | AAAA | O |
| ATOH | 3097 | H | LYS | 327 | 49.623 | 48.751 | 41.379 | 1.00 | 50.22 | AAAA | H |
| ATOH | 3099 | CA | LYS | 327 | 50.964 | 48.963 | 40.831 | 1.00 | 51.49 | AAAA | C |
| ATOH | 3100 | CB | LYS | 327 | 52.050 | 49.091 | 41.519 | 1.00 | 58.64 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|--------|------|---|
| ATOH | 3101 | CG | LYS | 327 | 53.254 | 48.827 | 41.981 | 1.00 | 59.15 | AAAA | C |
| ATOH | 3102 | CD | LYS | 327 | 54.528 | 48.257 | 41.617 | 1.00 | 63.49 | AAAA | C |
| ATOH | 3103 | CE | LYS | 327 | 55.400 | 48.951 | 40.592 | 1.00 | 68.12 | AAAA | C |
| ATOH | 3104 | ND | LYS | 327 | 56.260 | 47.889 | 39.938 | 1.00 | 71.97 | AAAA | H |
| ATOH | 3108 | C | LYS | 327 | 50.895 | 48.464 | 39.391 | 1.00 | 45.70 | AAAA | C |
| ATOH | 3109 | O | LYS | 327 | 50.901 | 47.245 | 39.127 | 1.00 | 49.55 | AAAA | O |
| ATOH | 3110 | H | GLY | 328 | 50.760 | 49.397 | 38.502 | 1.00 | 39.68 | AAAA | N |
| ATOH | 3112 | CA | GLY | 328 | 50.647 | 49.038 | 37.080 | 1.00 | 39.44 | AAAA | C |
| ATOH | 3113 | C | GLY | 328 | 49.845 | 50.161 | 36.427 | 1.00 | 39.49 | AAAA | C |
| ATOH | 3114 | O | GLY | 328 | 49.858 | 51.307 | 36.881 | 1.00 | 31.92 | AAAA | O |
| ATOH | 3115 | H | ASN | 329 | 49.286 | 49.813 | 35.289 | 1.00 | 41.47 | AAAA | N |
| ATOH | 3117 | CA | ASN | 329 | 48.467 | 50.750 | 34.543 | 1.00 | 45.72 | AAAA | C |
| ATOH | 3118 | CB | ASN | 329 | 49.185 | 50.842 | 33.211 | 1.00 | 42.50 | AAAA | C |
| ATOH | 3119 | CG | ASN | 329 | 50.624 | 51.426 | 33.357 | 1.00 | 42.26 | AAAA | C |
| ATOH | 3120 | OD1 | ASN | 329 | 50.954 | 52.331 | 34.156 | 1.00 | 34.77 | AAAA | O |
| ATOH | 3121 | ND2 | ASN | 329 | 51.425 | 50.769 | 32.530 | 1.00 | 30.62 | AAAA | H |
| ATOH | 3124 | C | ASN | 329 | 47.038 | 50.267 | 34.357 | 1.00 | 50.37 | AAAA | C |
| ATOH | 3125 | O | ASN | 329 | 46.736 | 49.015 | 34.119 | 1.00 | 50.17 | AAAA | O |
| ATOH | 3126 | H | LEU | 330 | 46.090 | 51.143 | 34.413 | 1.00 | 47.13 | AAAA | N |
| ATOH | 3128 | CA | LEU | 330 | 44.691 | 50.860 | 34.151 | 1.00 | 42.53 | AAAA | C |
| ATOH | 3129 | CB | LEU | 330 | 43.751 | 51.530 | 35.153 | 1.00 | 42.84 | AAAA | C |
| ATOH | 3130 | CG | LEU | 330 | 43.768 | 50.995 | 36.598 | 1.00 | 38.65 | AAAA | C |
| ATOH | 3131 | CD1 | LEU | 330 | 42.864 | 51.924 | 37.417 | 1.00 | 38.12 | AAAA | C |
| ATOH | 3132 | CD2 | LEU | 330 | 43.283 | 49.565 | 36.669 | 1.00 | 38.74 | AAAA | C |
| ATOH | 3133 | C | LEU | 330 | 44.352 | 51.377 | 32.758 | 1.00 | 39.10 | AAAA | C |
| ATOH | 3134 | O | LEU | 330 | 44.509 | 52.545 | 32.460 | 1.00 | 40.71 | AAAA | O |
| ATOH | 3135 | H | LEU | 331 | 43.933 | 50.516 | 31.904 | 1.00 | 36.10 | AAAA | N |
| ATOH | 3137 | CA | LEU | 331 | 43.367 | 50.869 | 30.625 | 1.00 | 43.10 | AAAA | C |
| ATOH | 3138 | CB | LEU | 331 | 43.958 | 49.894 | 29.585 | 1.00 | 42.29 | AAAA | C |
| ATOH | 3139 | CG | LEU | 331 | 43.301 | 49.960 | 28.221 | 1.00 | 40.89 | AAAA | C |
| ATOH | 3140 | CD1 | LEU | 331 | 43.501 | 51.319 | 27.627 | 1.00 | 46.64 | AAAA | C |
| ATOH | 3141 | CD2 | LEU | 331 | 43.844 | 48.834 | 27.367 | 1.00 | 48.76 | AAAA | C |
| ATOH | 3142 | C | LEU | 331 | 41.872 | 50.568 | 30.705 | 1.00 | 41.12 | AAAA | C |
| ATOH | 3143 | O | LEU | 331 | 41.562 | 49.365 | 30.779 | 1.00 | 40.08 | AAAA | O |
| ATOH | 3144 | H | ILE | 332 | 41.029 | 51.566 | 30.862 | 1.00 | 41.13 | AAAA | H |
| ATOH | 3146 | CA | ILE | 332 | 39.666 | 51.241 | 31.044 | 1.00 | 36.90 | AAAA | C |
| ATOH | 3147 | CB | ILE | 332 | 38.985 | 50.085 | 32.076 | 1.00 | 34.77 | AAAA | C |
| ATOH | 3148 | CG | ILE | 332 | 37.413 | 51.612 | 32.195 | 1.00 | 34.66 | AAAA | C |
| ATOH | 3149 | CD1 | ILE | 332 | 39.556 | 51.895 | 33.452 | 1.00 | 33.64 | AAAA | C |
| ATOH | 3150 | CD2 | ILE | 332 | 39.479 | 53.152 | 34.337 | 1.00 | 48.21 | AAAA | C |
| ATOH | 3151 | C | ILE | 332 | 38.959 | 51.367 | 29.689 | 1.00 | 34.03 | AAAA | C |
| ATOH | 3152 | O | ILE | 332 | 38.967 | 52.489 | 29.200 | 1.00 | 35.89 | AAAA | O |
| ATOH | 3153 | H | ASN | 333 | 38.569 | 53.273 | 29.094 | 1.00 | 35.25 | AAAA | H |
| ATOH | 3155 | CA | ASN | 333 | 38.014 | 50.293 | 27.737 | 1.00 | 40.34 | AAAA | C |
| ATOH | 3156 | CB | ASN | 333 | 38.960 | 49.499 | 26.797 | 1.00 | 50.50 | AAAA | C |
| ATOH | 3157 | CG | ASN | 333 | 36.669 | 49.493 | 25.310 | 1.00 | 59.29 | AAAA | C |
| ATOH | 3158 | OD1 | ASN | 333 | 37.845 | 48.711 | 24.784 | 1.00 | 64.54 | AAAA | O |
| ATOH | 3159 | ND2 | ASN | 333 | 39.290 | 50.350 | 24.467 | 1.00 | 45.83 | AAAA | H |
| ATOH | 3161 | C | ASN | 333 | 36.666 | 49.591 | 27.755 | 1.00 | 47.63 | AAAA | C |
| ATOH | 3163 | O | ASN | 333 | 36.462 | 48.409 | 27.399 | 1.00 | 44.40 | AAAA | O |
| ATOH | 3164 | H | ILE | 334 | 35.644 | 50.213 | 28.315 | 1.00 | 54.13 | AAAA | H |
| ATOH | 3166 | CA | ILE | 334 | 34.332 | 49.537 | 28.460 | 1.00 | 59.07 | AAAA | C |
| ATOH | 3167 | CB | ILE | 334 | 33.788 | 49.926 | 29.876 | 1.00 | 61.98 | AAAA | C |
| ATOH | 3168 | CG | ILE | 334 | 32.362 | 49.355 | 30.047 | 1.00 | 54.04 | AAAA | C |
| ATOH | 3169 | CD1 | ILE | 334 | 34.737 | 49.224 | 30.915 | 1.00 | 60.43 | AAAA | C |
| ATOH | 3170 | CD2 | ILE | 334 | 34.346 | 49.687 | 32.317 | 1.00 | 68.57 | AAAA | C |
| ATOH | 3171 | C | ILE | 334 | 33.271 | 50.032 | 27.476 | 1.00 | 59.45 | AAAA | C |
| ATOH | 3172 | O | ILE | 334 | 32.726 | 51.136 | 27.635 | 1.00 | 56.22 | AAAA | O |
| ATOH | 3173 | H | ARG | 335 | 32.919 | 49.181 | 26.550 | 1.00 | 59.69 | AAAA | N |
| ATOH | 3175 | CA | ARG | 335 | 31.910 | 49.567 | 25.573 | 1.00 | 73.93 | AAAA | C |
| ATOH | 3176 | CB | ARG | 335 | 32.262 | 49.903 | 24.240 | 1.00 | 74.44 | AAAA | C |
| ATOH | 3177 | CG | ARG | 335 | 33.729 | 48.932 | 23.918 | 1.00 | 82.97 | AAAA | C |
| ATOH | 3178 | CD | ARG | 335 | 34.102 | 49.289 | 22.500 | 1.00 | 86.49 | AAAA | C |
| ATOH | 3179 | NE | ARG | 335 | 34.361 | 49.040 | 21.777 | 1.00 | 89.83 | AAAA | N |
| ATOH | 3181 | CC | ARG | 335 | 34.011 | 47.838 | 20.496 | 1.00 | 93.67 | AAAA | C |
| ATOH | 3182 | HH1 | ARG | 335 | 33.409 | 48.852 | 19.843 | 1.00 | 87.24 | AAAA | H |
| ATOH | 3185 | HH2 | ARG | 335 | 34.256 | 46.674 | 19.877 | 1.00 | 75.31 | AAAA | N |
| ATOH | 3188 | C | ARG | 335 | 30.492 | 49.233 | 26.021 | 1.00 | 81.52 | AAAA | C |
| ATOH | 3189 | O | ARG | 335 | 29.664 | 50.115 | 26.239 | 1.00 | 84.11 | AAAA | O |
| ATOH | 3190 | H | ALA | 336 | 30.208 | 47.953 | 26.234 | 1.00 | 87.51 | AAAA | N |
| ATOH | 3192 | CA | ALA | 336 | 28.878 | 47.484 | 26.601 | 1.00 | 82.40 | AAAA | C |
| ATOH | 3193 | CB | ALA | 336 | 28.835 | 45.980 | 26.633 | 1.00 | 94.03 | AAAA | C |
| ATOH | 3194 | C | ALA | 336 | 28.479 | 48.058 | 27.953 | 1.00 | 96.61 | AAAA | C |
| ATOH | 3195 | O | ALA | 336 | 29.316 | 48.019 | 28.855 | 1.00 | 96.96 | AAAA | O |
| ATOH | 3196 | H | GLY | 337 | 27.298 | 48.685 | 28.039 | 1.00 | 99.74 | AAAA | N |
| ATOH | 3199 | CA | GLY | 337 | 26.986 | 49.385 | 29.272 | 1.00 | 103.11 | AAAA | C |
| ATOH | 3199 | C | GLY | 337 | 25.568 | 49.303 | 29.763 | 1.00 | 105.51 | AAAA | C |
| ATOH | 3200 | O | GLY | 337 | 24.801 | 50.267 | 29.596 | 1.00 | 106.64 | AAAA | O |
| ATOH | 3201 | H | ASN | 338 | 25.243 | 48.146 | 30.346 | 1.00 | 105.41 | AAAA | N |
| ATOH | 3203 | CA | ASN | 338 | 23.886 | 49.017 | 30.908 | 1.00 | 106.92 | AAAA | C |
| ATOH | 3204 | CB | ASN | 338 | 23.714 | 46.689 | 31.624 | 1.00 | 109.14 | AAAA | C |
| ATOH | 3205 | CG | ASN | 338 | 24.403 | 45.544 | 30.928 | 1.00 | 112.30 | AAAA | C |
| ATOH | 3206 | OD1 | ASN | 338 | 25.598 | 45.595 | 30.625 | 1.00 | 117.94 | AAAA | O |
| ATOH | 3207 | ND2 | ASN | 338 | 23.604 | 44.508 | 30.683 | 1.00 | 113.72 | AAAA | N |
| ATOH | 3210 | C | ASN | 338 | 23.790 | 49.160 | 31.931 | 1.00 | 105.84 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------------|------|---|
| ATOH | 3211 | O | ASH | 338 | 23.544 | 50.345 | 31.739 | 1.00103.97 | AAAA | O |
| ATOH | 3212 | H | ASH | 339 | 24.290 | 48.762 | 33.099 | 1.00105.47 | AAAA | H |
| ATOH | 3214 | CA | ASH | 339 | 24.529 | 49.740 | 34.159 | 1.00107.10 | AAAA | C |
| ATOH | 3215 | CB | ASH | 339 | 23.252 | 49.915 | 34.945 | 1.00109.15 | AAAA | C |
| ATOH | 3216 | CG | ASH | 339 | 22.777 | 51.351 | 35.003 | 0.01107.52 | AAAA | C |
| ATOH | 3217 | OD1 | ASH | 339 | 22.715 | 51.931 | 36.088 | 0.01107.49 | AAAA | O |
| ATOH | 3218 | HD2 | ASH | 339 | 22.441 | 51.932 | 33.859 | 0.01107.46 | AAAA | H |
| ATOH | 3221 | C | ASH | 339 | 25.697 | 49.237 | 35.007 | 1.00106.33 | AAAA | C |
| ATOH | 3222 | O | ASH | 339 | 25.520 | 48.390 | 35.886 | 1.00108.82 | AAAA | O |
| ATOH | 3223 | H | ILE | 340 | 26.897 | 49.527 | 34.510 | 1.00101.36 | AAAA | H |
| ATOH | 3225 | CA | ILE | 340 | 28.136 | 49.101 | 35.138 | 1.00 97.43 | AAAA | C |
| ATOH | 3226 | CB | ILE | 340 | 29.040 | 48.354 | 34.151 | 1.00 93.63 | AAAA | C |
| ATOH | 3227 | CG | ILE | 340 | 28.194 | 47.252 | 33.489 | 1.00 99.38 | AAAA | C |
| ATOH | 3229 | OG1 | ILE | 340 | 29.726 | 49.158 | 33.070 | 1.00 85.50 | AAAA | C |
| ATOH | 3229 | OD1 | ILE | 340 | 28.897 | 49.634 | 31.915 | 1.00 92.53 | AAAA | C |
| ATOH | 3230 | C | ILE | 340 | 28.783 | 50.357 | 35.706 | 1.00 95.32 | AAAA | C |
| ATOH | 3231 | O | ILE | 340 | 29.472 | 51.099 | 34.997 | 1.00 97.86 | AAAA | O |
| ATOH | 3232 | H | ALA | 341 | 28.409 | 50.739 | 36.915 | 1.00 89.89 | AAAA | H |
| ATOH | 3234 | CA | ALA | 341 | 28.892 | 52.008 | 37.450 | 1.00 88.45 | AAAA | C |
| ATOH | 3235 | CB | ALA | 341 | 28.068 | 53.201 | 37.006 | 1.00 84.56 | AAAA | C |
| ATOH | 3236 | C | ALA | 341 | 28.786 | 51.968 | 38.970 | 1.00 85.37 | AAAA | C |
| ATOH | 3237 | O | ALA | 341 | 28.910 | 52.935 | 39.690 | 1.00 86.09 | AAAA | O |
| ATOH | 3238 | H | SER | 342 | 28.204 | 50.877 | 39.386 | 1.00 84.24 | AAAA | N |
| ATOH | 3240 | CA | SER | 342 | 27.910 | 50.601 | 40.780 | 1.00 82.05 | AAAA | C |
| ATOH | 3241 | CB | SER | 342 | 26.426 | 50.667 | 41.112 | 1.00 85.51 | AAAA | C |
| ATOH | 3242 | CG | SER | 342 | 26.145 | 51.271 | 42.361 | 1.00 86.02 | AAAA | C |
| ATOH | 3244 | C | SER | 342 | 28.487 | 49.196 | 40.965 | 1.00 76.62 | AAAA | C |
| ATOH | 3245 | O | SER | 342 | 29.119 | 48.966 | 41.964 | 1.00 71.76 | AAAA | O |
| ATOH | 3246 | H | GLU | 343 | 28.373 | 48.409 | 39.905 | 1.00 76.23 | AAAA | H |
| ATOH | 3248 | CA | GLU | 343 | 29.001 | 47.109 | 39.820 | 1.00 74.59 | AAAA | C |
| ATOH | 3249 | CB | GLU | 343 | 28.595 | 46.300 | 38.616 | 1.00 78.62 | AAAA | C |
| ATOH | 3250 | CG | GLU | 343 | 27.118 | 46.105 | 38.316 | 1.00 85.33 | AAAA | C |
| ATOH | 3251 | OD | GLU | 343 | 26.898 | 45.121 | 37.169 | 1.00 92.76 | AAAA | C |
| ATOH | 3252 | OE1 | GLU | 343 | 27.209 | 43.911 | 37.310 | 1.00 96.41 | AAAA | O |
| ATOH | 3253 | OE2 | GLU | 343 | 26.423 | 45.517 | 36.082 | 1.00 98.55 | AAAA | O |
| ATOH | 3254 | C | GLU | 343 | 30.525 | 47.319 | 39.804 | 1.00 77.75 | AAAA | C |
| ATOH | 3255 | O | GLU | 343 | 31.273 | 46.797 | 40.637 | 1.00 75.73 | AAAA | O |
| ATOH | 3256 | H | LEU | 344 | 31.022 | 49.237 | 39.965 | 1.00 75.65 | AAAA | H |
| ATOH | 3258 | CA | LEU | 344 | 32.415 | 48.596 | 38.833 | 1.00 72.36 | AAAA | C |
| ATOH | 3259 | CB | LEU | 344 | 32.760 | 49.697 | 37.809 | 1.00 64.33 | AAAA | C |
| ATOH | 3261 | CG | LEU | 344 | 32.687 | 49.397 | 36.311 | 1.00 50.12 | AAAA | C |
| ATOH | 3261 | OD1 | LEU | 344 | 33.224 | 50.577 | 35.519 | 1.00 57.00 | AAAA | C |
| ATOH | 3262 | OD2 | LEU | 344 | 33.401 | 48.127 | 35.905 | 1.00 51.62 | AAAA | C |
| ATOH | 3263 | C | LEU | 344 | 32.963 | 49.130 | 40.174 | 1.00 69.74 | AAAA | C |
| ATOH | 3264 | O | LEU | 344 | 34.079 | 48.739 | 40.551 | 1.00 69.12 | AAAA | O |
| ATOH | 3265 | H | LEU | 345 | 32.166 | 49.959 | 40.822 | 1.00 63.10 | AAAA | H |
| ATOH | 3267 | CA | LEU | 345 | 32.555 | 50.891 | 42.061 | 1.00 65.42 | AAAA | C |
| ATOH | 3268 | CB | LEU | 345 | 31.592 | 51.714 | 42.478 | 1.00 55.59 | AAAA | C |
| ATOH | 3269 | CG | LEU | 345 | 32.267 | 52.607 | 43.486 | 1.00 68.78 | AAAA | C |
| ATOH | 3271 | OD | LEU | 345 | 31.324 | 53.374 | 44.376 | 1.00 81.31 | AAAA | C |
| ATOH | 3271 | OE1 | LEU | 345 | 30.614 | 54.320 | 43.976 | 1.00 85.60 | AAAA | O |
| ATOH | 3272 | OE2 | LEU | 345 | 31.237 | 53.078 | 45.595 | 1.00 88.79 | AAAA | O |
| ATOH | 3273 | C | LEU | 345 | 32.706 | 49.652 | 43.255 | 1.00 63.31 | AAAA | C |
| ATOH | 3274 | O | LEU | 345 | 33.501 | 49.913 | 44.134 | 1.00 60.06 | AAAA | O |
| ATOH | 3275 | H | ASH | 346 | 32.151 | 48.462 | 43.202 | 1.00 62.25 | AAAA | H |
| ATOH | 3277 | CA | ASH | 346 | 32.285 | 47.403 | 44.173 | 1.00 63.82 | AAAA | C |
| ATOH | 3279 | CB | ASH | 346 | 31.024 | 46.498 | 44.095 | 1.00 61.66 | AAAA | C |
| ATOH | 3279 | CG | ASH | 346 | 31.110 | 45.292 | 45.006 | 1.00 58.73 | AAAA | C |
| ATOH | 3290 | OD1 | ASH | 346 | 31.188 | 45.352 | 46.224 | 1.00 69.11 | AAAA | O |
| ATOH | 3281 | HD2 | ASH | 346 | 31.155 | 44.092 | 44.444 | 1.00 51.10 | AAAA | H |
| ATOH | 3294 | C | ASH | 346 | 33.532 | 46.580 | 43.870 | 1.00 63.71 | AAAA | C |
| ATOH | 3295 | O | ASH | 346 | 33.636 | 45.336 | 43.905 | 1.00 65.65 | AAAA | O |
| ATOH | 3296 | H | PHE | 347 | 34.419 | 47.173 | 43.066 | 1.00 63.23 | AAAA | N |
| ATOH | 3298 | CA | PHE | 347 | 35.540 | 46.411 | 42.506 | 1.00 61.39 | AAAA | C |
| ATOH | 3299 | CB | PHE | 347 | 35.123 | 45.854 | 41.170 | 1.00 61.38 | AAAA | C |
| ATOH | 3290 | CG | PHE | 347 | 34.457 | 44.534 | 41.142 | 1.00 65.57 | AAAA | C |
| ATOH | 3291 | OD1 | PHE | 347 | 33.090 | 44.438 | 40.982 | 1.00 75.25 | AAAA | C |
| ATOH | 3292 | OD2 | PHE | 347 | 35.148 | 43.351 | 41.267 | 1.00 77.15 | AAAA | C |
| ATOH | 3293 | CE1 | PHE | 347 | 32.425 | 43.224 | 40.951 | 1.00 75.55 | AAAA | C |
| ATOH | 3294 | CE2 | PHE | 347 | 34.512 | 42.130 | 41.249 | 1.00 72.86 | AAAA | C |
| ATOH | 3295 | CG | PHE | 347 | 33.152 | 42.051 | 41.095 | 1.00 72.74 | AAAA | C |
| ATOH | 3296 | C | PHE | 347 | 36.712 | 47.375 | 42.440 | 1.00 57.70 | AAAA | C |
| ATOH | 3297 | O | PHE | 347 | 37.770 | 46.920 | 42.354 | 1.00 59.92 | AAAA | O |
| ATOH | 3299 | H | NET | 348 | 36.492 | 48.676 | 42.319 | 1.00 50.56 | AAAA | N |
| ATOH | 3300 | CA | NET | 348 | 37.500 | 49.630 | 41.964 | 1.00 42.86 | AAAA | C |
| ATOH | 3301 | CB | NET | 348 | 37.402 | 50.096 | 40.493 | 1.00 31.72 | AAAA | C |
| ATOH | 3302 | CG | NET | 348 | 37.426 | 48.933 | 39.471 | 1.00 33.42 | AAAA | C |
| ATOH | 3303 | SD | NET | 348 | 37.566 | 49.448 | 37.732 | 1.00 44.79 | AAAA | S |
| ATOH | 3304 | CE | NET | 348 | 38.408 | 50.999 | 37.791 | 1.00 59.57 | AAAA | C |
| ATOH | 3305 | C | NET | 348 | 37.368 | 50.831 | 42.867 | 1.00 45.88 | AAAA | C |
| ATOH | 3306 | O | NET | 348 | 38.210 | 51.772 | 42.901 | 1.00 43.33 | AAAA | O |
| ATOH | 3307 | H | GLY | 349 | 36.296 | 50.783 | 43.683 | 1.00 45.30 | AAAA | H |
| ATOH | 3309 | CA | GLY | 349 | 35.998 | 51.965 | 44.504 | 1.00 49.19 | AAAA | C |
| ATOH | 3310 | C | GLY | 349 | 36.980 | 52.189 | 45.620 | 1.00 52.77 | AAAA | C |
| ATOH | 3311 | O | GLY | 349 | 37.033 | 53.299 | 46.156 | 1.00 53.43 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 3312 | H | LEU | 350 | 37.791 | 51.159 | 45.925 | 1.00 | 56.17 | AAAA | H |
| ATOM | 3314 | CA | LEU | 350 | 38.735 | 51.256 | 47.021 | 1.00 | 58.04 | AAAA | C |
| ATOM | 3315 | CB | LEU | 350 | 38.873 | 49.949 | 47.834 | 1.00 | 49.00 | AAAA | C |
| ATOM | 3316 | CG | LEU | 350 | 37.871 | 50.020 | 49.031 | 1.00 | 50.79 | AAAA | C |
| ATOM | 3317 | CD1 | LEU | 350 | 37.705 | 48.680 | 49.700 | 1.00 | 52.92 | AAAA | C |
| ATOM | 3318 | CD2 | LEU | 350 | 38.247 | 51.106 | 50.038 | 1.00 | 56.11 | AAAA | C |
| ATOM | 3319 | C | LEU | 350 | 40.144 | 51.727 | 46.685 | 1.00 | 61.34 | AAAA | C |
| ATOM | 3320 | O | LEU | 350 | 40.931 | 51.962 | 47.618 | 1.00 | 63.52 | AAAA | O |
| ATOM | 3321 | H | ILE | 351 | 40.446 | 51.677 | 45.372 | 1.00 | 57.89 | AAAA | H |
| ATOM | 3323 | CA | ILE | 351 | 41.729 | 52.088 | 44.873 | 1.00 | 48.69 | AAAA | C |
| ATOM | 3324 | CB | ILE | 351 | 41.814 | 51.912 | 43.352 | 1.00 | 48.19 | AAAA | C |
| ATOM | 3325 | CG2 | ILE | 351 | 43.121 | 52.416 | 42.757 | 1.00 | 40.01 | AAAA | C |
| ATOM | 3326 | CG1 | ILE | 351 | 41.535 | 50.418 | 43.058 | 1.00 | 36.87 | AAAA | C |
| ATOM | 3327 | CD1 | ILE | 351 | 41.172 | 50.351 | 41.581 | 1.00 | 36.46 | AAAA | C |
| ATOM | 3328 | C | ILE | 351 | 42.031 | 53.533 | 45.178 | 1.00 | 46.80 | AAAA | C |
| ATOM | 3329 | O | ILE | 351 | 41.367 | 54.358 | 44.626 | 1.00 | 42.87 | AAAA | O |
| ATOM | 3330 | H | GLU | 352 | 43.002 | 53.866 | 46.015 | 1.00 | 50.61 | AAAA | H |
| ATOM | 3332 | CA | GLU | 352 | 43.381 | 55.241 | 46.248 | 1.00 | 51.20 | AAAA | C |
| ATOM | 3333 | CB | GLU | 352 | 43.907 | 55.353 | 47.678 | 1.00 | 52.12 | AAAA | C |
| ATOM | 3334 | CG | GLU | 352 | 42.912 | 55.769 | 48.735 | 1.00 | 65.55 | AAAA | C |
| ATOM | 3335 | CD | GLU | 352 | 43.034 | 54.834 | 49.947 | 1.00 | 71.49 | AAAA | C |
| ATOM | 3336 | OE1 | GLU | 352 | 43.881 | 55.244 | 50.765 | 1.00 | 66.09 | AAAA | O |
| ATOM | 3337 | OE2 | GLU | 352 | 42.330 | 53.799 | 50.009 | 1.00 | 76.07 | AAAA | O |
| ATOM | 3338 | C | GLU | 352 | 44.502 | 55.751 | 45.314 | 1.00 | 47.43 | AAAA | C |
| ATOM | 3339 | O | GLU | 352 | 44.798 | 56.951 | 45.182 | 1.00 | 40.38 | AAAA | O |
| ATOM | 3340 | H | VAL | 353 | 45.342 | 54.838 | 44.852 | 1.00 | 43.54 | AAAA | N |
| ATOM | 3342 | CA | VAL | 353 | 46.512 | 55.236 | 44.078 | 1.00 | 43.71 | AAAA | C |
| ATOM | 3343 | CB | VAL | 353 | 47.759 | 55.540 | 44.911 | 1.00 | 45.01 | AAAA | C |
| ATOM | 3344 | CG1 | VAL | 353 | 47.766 | 55.261 | 46.387 | 1.00 | 30.84 | AAAA | C |
| ATOM | 3345 | CG2 | VAL | 353 | 48.988 | 54.844 | 44.310 | 1.00 | 42.55 | AAAA | C |
| ATOM | 3346 | C | VAL | 353 | 46.828 | 54.233 | 42.957 | 1.00 | 41.41 | AAAA | C |
| ATOM | 3347 | O | VAL | 353 | 46.843 | 53.003 | 43.172 | 1.00 | 39.19 | AAAA | O |
| ATOM | 3348 | H | VAL | 354 | 47.074 | 54.855 | 41.816 | 1.00 | 36.31 | AAAA | H |
| ATOM | 3350 | CA | VAL | 354 | 47.586 | 54.092 | 40.651 | 1.00 | 43.97 | AAAA | C |
| ATOM | 3351 | CB | VAL | 354 | 46.725 | 54.390 | 39.407 | 1.00 | 40.96 | AAAA | C |
| ATOM | 3352 | CG1 | VAL | 354 | 47.347 | 53.896 | 38.123 | 1.00 | 36.72 | AAAA | C |
| ATOM | 3353 | CG2 | VAL | 354 | 45.293 | 53.849 | 39.678 | 1.00 | 35.35 | AAAA | C |
| ATOM | 3354 | C | VAL | 354 | 49.043 | 54.510 | 40.388 | 1.00 | 44.56 | AAAA | C |
| ATOM | 3355 | O | VAL | 354 | 49.366 | 55.718 | 40.288 | 1.00 | 43.32 | AAAA | O |
| ATOM | 3356 | H | THR | 355 | 49.972 | 53.561 | 40.431 | 1.00 | 43.93 | AAAA | H |
| ATOM | 3358 | CA | THR | 355 | 51.392 | 53.914 | 40.284 | 1.00 | 44.85 | AAAA | C |
| ATOM | 3359 | CB | THR | 355 | 52.374 | 52.799 | 40.653 | 1.00 | 42.40 | AAAA | C |
| ATOM | 3360 | CG1 | THR | 355 | 52.273 | 51.744 | 39.695 | 1.00 | 45.30 | AAAA | O |
| ATOM | 3362 | CG2 | THR | 355 | 52.210 | 52.194 | 42.039 | 1.00 | 38.13 | AAAA | C |
| ATOM | 3363 | C | THR | 355 | 51.746 | 54.339 | 38.851 | 1.00 | 43.84 | AAAA | C |
| ATOM | 3364 | O | THR | 355 | 52.463 | 55.334 | 38.697 | 1.00 | 44.26 | AAAA | O |
| ATOM | 3365 | H | GLY | 356 | 51.127 | 53.704 | 37.870 | 1.00 | 41.16 | AAAA | H |
| ATOM | 3367 | CA | GLY | 356 | 51.358 | 54.073 | 36.470 | 1.00 | 37.81 | AAAA | C |
| ATOM | 3368 | C | GLY | 356 | 50.505 | 53.004 | 35.955 | 1.00 | 38.07 | AAAA | C |
| ATOM | 3369 | O | GLY | 356 | 50.364 | 56.261 | 36.615 | 1.00 | 34.65 | AAAA | O |
| ATOM | 3370 | H | TYR | 357 | 49.910 | 55.004 | 34.800 | 1.00 | 38.47 | AAAA | H |
| ATOM | 3372 | CA | TYR | 357 | 49.982 | 55.973 | 34.205 | 1.00 | 38.03 | AAAA | C |
| ATOM | 3373 | CB | TYR | 357 | 49.557 | 56.343 | 32.905 | 1.00 | 31.44 | AAAA | C |
| ATOM | 3374 | CG | TYR | 357 | 49.473 | 55.219 | 31.812 | 1.00 | 33.04 | AAAA | C |
| ATOM | 3375 | CD1 | TYR | 357 | 48.333 | 54.842 | 31.077 | 1.00 | 32.86 | AAAA | C |
| ATOM | 3376 | CE1 | TYR | 357 | 48.352 | 53.779 | 30.175 | 1.00 | 32.83 | AAAA | C |
| ATOM | 3377 | CD2 | TYR | 357 | 50.639 | 54.465 | 31.606 | 1.00 | 34.28 | AAAA | C |
| ATOM | 3378 | CE2 | TYR | 357 | 50.706 | 53.402 | 30.720 | 1.00 | 32.51 | AAAA | C |
| ATOM | 3379 | CE | TYR | 357 | 49.552 | 53.068 | 30.007 | 1.00 | 37.26 | AAAA | C |
| ATOM | 3380 | OH | TYR | 357 | 49.726 | 51.997 | 29.166 | 1.00 | 35.85 | AAAA | O |
| ATOM | 3382 | C | TYR | 357 | 47.582 | 55.368 | 34.150 | 1.00 | 38.55 | AAAA | C |
| ATOM | 3383 | O | TYR | 357 | 47.458 | 54.127 | 34.088 | 1.00 | 36.11 | AAAA | O |
| ATOM | 3384 | H | VAL | 358 | 46.593 | 56.216 | 33.814 | 1.00 | 40.98 | AAAA | H |
| ATOM | 3386 | CA | VAL | 358 | 45.197 | 55.798 | 33.639 | 1.00 | 38.90 | AAAA | C |
| ATOM | 3387 | CB | VAL | 358 | 44.211 | 56.502 | 34.610 | 1.00 | 49.15 | AAAA | C |
| ATOM | 3388 | CG1 | VAL | 358 | 42.815 | 55.883 | 34.484 | 1.00 | 33.12 | AAAA | C |
| ATOM | 3389 | CG2 | VAL | 358 | 44.748 | 56.437 | 36.043 | 1.00 | 29.20 | AAAA | C |
| ATOM | 3390 | C | VAL | 358 | 44.760 | 56.194 | 32.234 | 1.00 | 35.64 | AAAA | C |
| ATOM | 3391 | O | VAL | 358 | 44.792 | 57.358 | 31.888 | 1.00 | 34.58 | AAAA | O |
| ATOM | 3392 | H | LYS | 359 | 44.387 | 55.188 | 31.461 | 1.00 | 36.00 | AAAA | H |
| ATOM | 3394 | CA | LYS | 359 | 43.898 | 55.419 | 30.117 | 1.00 | 41.27 | AAAA | C |
| ATOM | 3395 | CB | LYS | 359 | 44.845 | 54.707 | 29.174 | 1.00 | 37.40 | AAAA | C |
| ATOM | 3396 | CG | LYS | 359 | 44.340 | 54.473 | 27.770 | 1.00 | 45.19 | AAAA | C |
| ATOM | 3397 | CD | LYS | 359 | 45.040 | 55.317 | 26.750 | 1.00 | 43.40 | AAAA | C |
| ATOM | 3398 | CE | LYS | 359 | 45.958 | 54.402 | 25.986 | 1.00 | 43.56 | AAAA | C |
| ATOM | 3399 | HE | LYS | 359 | 45.416 | 53.937 | 24.680 | 1.00 | 47.98 | AAAA | H |
| ATOM | 3403 | C | LYS | 359 | 42.423 | 54.979 | 29.939 | 1.00 | 42.14 | AAAA | C |
| ATOM | 3404 | O | LYS | 359 | 42.056 | 53.791 | 30.006 | 1.00 | 40.40 | AAAA | O |
| ATOM | 3405 | H | ILE | 360 | 41.602 | 55.974 | 29.572 | 1.00 | 37.16 | AAAA | H |
| ATOM | 3407 | CA | ILE | 360 | 40.164 | 55.742 | 29.334 | 1.00 | 40.02 | AAAA | C |
| ATOM | 3408 | CB | ILE | 360 | 39.297 | 56.804 | 30.048 | 1.00 | 38.10 | AAAA | C |
| ATOM | 3409 | CG2 | ILE | 360 | 37.887 | 56.277 | 29.932 | 1.00 | 39.42 | AAAA | C |
| ATOM | 3410 | CG1 | ILE | 360 | 39.769 | 57.111 | 31.481 | 1.00 | 28.54 | AAAA | C |
| ATOM | 3411 | CD1 | ILE | 360 | 39.423 | 56.037 | 32.491 | 1.00 | 33.16 | AAAA | C |
| ATOM | 3412 | C | ILE | 360 | 39.888 | 55.837 | 27.834 | 1.00 | 39.49 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 3413 | O | ILE | 360 | 40.014 | 56.942 | 27.235 | 1.00 | 37.32 | AAAA | O |
| ATOM | 3414 | H | ARG | 361 | 39.567 | 54.721 | 27.221 | 1.00 | 34.34 | AAAA | H |
| ATOM | 3416 | CA | ARG | 361 | 39.472 | 54.782 | 25.744 | 1.00 | 41.24 | AAAA | C |
| ATOM | 3417 | CB | ARG | 361 | 40.783 | 54.213 | 25.148 | 1.00 | 47.92 | AAAA | C |
| ATOM | 3418 | CG | ARG | 361 | 40.805 | 54.203 | 23.646 | 1.00 | 50.39 | AAAA | C |
| ATOM | 3419 | CD | ARG | 361 | 41.943 | 53.357 | 23.116 | 1.00 | 51.36 | AAAA | C |
| ATOM | 3420 | HE | ARG | 361 | 41.473 | 51.974 | 23.263 | 1.00 | 50.97 | AAAA | H |
| ATOM | 3422 | CE | ARG | 361 | 42.297 | 50.962 | 23.490 | 1.00 | 55.78 | AAAA | C |
| ATOM | 3423 | HH1 | ARG | 361 | 43.612 | 51.074 | 23.616 | 1.00 | 51.62 | AAAA | H |
| ATOM | 3426 | HH2 | ARG | 361 | 41.834 | 49.719 | 23.631 | 1.00 | 54.52 | AAAA | H |
| ATOM | 3429 | C | ARG | 361 | 38.382 | 53.866 | 25.246 | 1.00 | 42.06 | AAAA | C |
| ATOM | 3430 | O | ARG | 361 | 38.336 | 52.661 | 25.499 | 1.00 | 38.93 | AAAA | O |
| ATOM | 3431 | H | HIS | 362 | 37.514 | 54.342 | 24.373 | 1.00 | 46.19 | AAAA | H |
| ATOM | 3433 | CA | HIS | 362 | 36.372 | 53.555 | 23.885 | 1.00 | 49.34 | AAAA | C |
| ATOM | 3434 | CB | HIS | 362 | 37.000 | 52.300 | 23.266 | 1.00 | 40.94 | AAAA | C |
| ATOM | 3435 | CG | HIS | 362 | 37.849 | 52.610 | 22.084 | 1.00 | 42.78 | AAAA | C |
| ATOM | 3436 | CD2 | HIS | 362 | 38.049 | 53.765 | 21.411 | 1.00 | 48.32 | AAAA | C |
| ATOM | 3437 | HD1 | HIS | 362 | 38.628 | 51.676 | 21.469 | 1.00 | 43.59 | AAAA | H |
| ATOM | 3439 | CE1 | HIS | 362 | 39.256 | 52.247 | 20.465 | 1.00 | 46.01 | AAAA | C |
| ATOM | 3440 | HE2 | HIS | 362 | 38.923 | 53.515 | 20.408 | 1.00 | 49.22 | AAAA | H |
| ATOM | 3442 | C | HIS | 362 | 35.295 | 53.113 | 24.913 | 1.00 | 50.32 | AAAA | C |
| ATOM | 3443 | O | HIS | 362 | 34.686 | 52.030 | 24.795 | 1.00 | 41.31 | AAAA | O |
| ATOM | 3444 | H | SER | 363 | 35.222 | 53.875 | 26.013 | 1.00 | 46.96 | AAAA | H |
| ATOM | 3446 | CA | SER | 363 | 34.402 | 53.456 | 27.139 | 1.00 | 52.19 | AAAA | C |
| ATOM | 3447 | CB | SER | 363 | 35.231 | 53.837 | 28.400 | 1.00 | 53.73 | AAAA | C |
| ATOM | 3448 | CG | SER | 363 | 35.713 | 52.558 | 28.816 | 1.00 | 41.72 | AAAA | C |
| ATOM | 3450 | C | SER | 363 | 33.005 | 54.072 | 27.046 | 1.00 | 49.08 | AAAA | C |
| ATOM | 3451 | O | SER | 363 | 32.653 | 55.040 | 27.694 | 1.00 | 37.49 | AAAA | O |
| ATOM | 3452 | H | HIS | 364 | 32.243 | 53.577 | 26.058 | 1.00 | 52.25 | AAAA | H |
| ATOM | 3454 | CA | HIS | 364 | 30.954 | 54.173 | 25.717 | 1.00 | 53.66 | AAAA | C |
| ATOM | 3455 | C | HIS | 364 | 29.879 | 53.937 | 26.760 | 1.00 | 48.77 | AAAA | C |
| ATOM | 3456 | O | HIS | 364 | 29.297 | 54.899 | 27.280 | 1.00 | 51.44 | AAAA | O |
| ATOM | 3457 | CB | HIS | 364 | 30.485 | 53.699 | 24.348 | 1.00 | 49.83 | AAAA | C |
| ATOM | 3458 | CG | HIS | 364 | 31.493 | 54.182 | 23.339 | 1.00 | 51.51 | AAAA | C |
| ATOM | 3459 | HD1 | HIS | 364 | 31.870 | 55.502 | 23.156 | 1.00 | 44.83 | AAAA | H |
| ATOM | 3460 | CE1 | HIS | 364 | 32.798 | 55.533 | 22.214 | 1.00 | 28.57 | AAAA | C |
| ATOM | 3461 | CD2 | HIS | 364 | 32.194 | 53.393 | 22.472 | 1.00 | 38.62 | AAAA | C |
| ATOM | 3462 | HE2 | HIS | 364 | 32.992 | 54.274 | 21.810 | 1.00 | 41.44 | AAAA | H |
| ATOM | 3464 | H | ALA | 365 | 29.949 | 52.819 | 27.427 | 1.00 | 47.53 | AAAA | H |
| ATOM | 3466 | CA | ALA | 365 | 29.211 | 52.488 | 28.621 | 1.00 | 44.41 | AAAA | C |
| ATOM | 3467 | CB | ALA | 365 | 29.678 | 51.133 | 29.150 | 1.00 | 40.28 | AAAA | C |
| ATOM | 3468 | C | ALA | 365 | 29.318 | 53.473 | 29.768 | 1.00 | 44.70 | AAAA | C |
| ATOM | 3469 | O | ALA | 365 | 28.576 | 53.206 | 30.726 | 1.00 | 45.28 | AAAA | O |
| ATOM | 3470 | H | LEU | 366 | 30.158 | 54.517 | 29.762 | 1.00 | 40.80 | AAAA | H |
| ATOM | 3472 | CA | LEU | 366 | 30.415 | 55.243 | 30.969 | 1.00 | 42.21 | AAAA | C |
| ATOM | 3473 | CB | LEU | 366 | 31.985 | 55.241 | 31.350 | 1.00 | 43.79 | AAAA | C |
| ATOM | 3474 | CG | LEU | 366 | 32.740 | 54.037 | 31.667 | 1.00 | 51.52 | AAAA | C |
| ATOM | 3475 | CD1 | LEU | 366 | 34.192 | 54.373 | 32.043 | 1.00 | 51.77 | AAAA | C |
| ATOM | 3476 | CD2 | LEU | 366 | 32.118 | 53.305 | 32.834 | 1.00 | 51.17 | AAAA | C |
| ATOM | 3477 | C | LEU | 366 | 29.974 | 56.687 | 30.896 | 1.00 | 46.35 | AAAA | C |
| ATOM | 3478 | O | LEU | 366 | 30.305 | 57.248 | 29.849 | 1.00 | 48.40 | AAAA | O |
| ATOM | 3479 | H | VAL | 367 | 29.521 | 57.275 | 32.015 | 1.00 | 43.68 | AAAA | H |
| ATOM | 3481 | CA | VAL | 367 | 29.072 | 58.675 | 31.940 | 1.00 | 44.18 | AAAA | C |
| ATOM | 3482 | CB | VAL | 367 | 27.557 | 58.727 | 32.376 | 1.00 | 48.80 | AAAA | C |
| ATOM | 3483 | CG1 | VAL | 367 | 26.923 | 60.073 | 32.571 | 1.00 | 41.69 | AAAA | C |
| ATOM | 3484 | CG2 | VAL | 367 | 26.697 | 57.949 | 31.365 | 1.00 | 34.00 | AAAA | C |
| ATOM | 3485 | C | VAL | 367 | 29.923 | 59.518 | 32.845 | 1.00 | 44.90 | AAAA | C |
| ATOM | 3486 | O | VAL | 367 | 29.965 | 60.751 | 32.720 | 1.00 | 44.75 | AAAA | O |
| ATOM | 3487 | H | SER | 368 | 30.591 | 58.818 | 33.757 | 1.00 | 48.72 | AAAA | H |
| ATOM | 3489 | CA | SER | 368 | 31.487 | 59.465 | 34.742 | 1.00 | 52.70 | AAAA | C |
| ATOM | 3490 | CB | SER | 368 | 30.658 | 59.706 | 36.000 | 1.00 | 55.32 | AAAA | C |
| ATOM | 3491 | CG | SER | 368 | 31.300 | 60.298 | 37.091 | 1.00 | 64.86 | AAAA | C |
| ATOM | 3493 | C | SER | 368 | 32.590 | 58.497 | 35.179 | 1.00 | 52.76 | AAAA | C |
| ATOM | 3494 | O | SER | 368 | 32.352 | 57.299 | 34.976 | 1.00 | 48.99 | AAAA | O |
| ATOM | 3495 | H | LEU | 369 | 33.631 | 59.012 | 35.831 | 1.00 | 53.86 | AAAA | H |
| ATOM | 3497 | CA | LEU | 369 | 34.716 | 58.129 | 36.274 | 1.00 | 60.15 | AAAA | C |
| ATOM | 3498 | CB | LEU | 369 | 36.073 | 58.630 | 35.784 | 1.00 | 55.91 | AAAA | C |
| ATOM | 3499 | CG | LEU | 369 | 36.325 | 58.736 | 34.271 | 1.00 | 45.96 | AAAA | C |
| ATOM | 3500 | CD1 | LEU | 369 | 37.669 | 59.428 | 34.154 | 1.00 | 53.97 | AAAA | C |
| ATOM | 3501 | CD2 | LEU | 369 | 36.207 | 57.384 | 33.619 | 1.00 | 38.77 | AAAA | C |
| ATOM | 3502 | C | LEU | 369 | 34.645 | 58.036 | 37.811 | 1.00 | 62.52 | AAAA | C |
| ATOM | 3503 | O | LEU | 369 | 35.569 | 57.700 | 38.595 | 1.00 | 59.33 | AAAA | O |
| ATOM | 3504 | H | SER | 370 | 33.437 | 58.401 | 38.285 | 1.00 | 56.26 | AAAA | H |
| ATOM | 3506 | CA | SER | 370 | 33.089 | 58.431 | 39.690 | 1.00 | 53.89 | AAAA | C |
| ATOM | 3507 | CB | SER | 370 | 31.673 | 59.052 | 39.816 | 1.00 | 57.50 | AAAA | C |
| ATOM | 3508 | CG | SER | 370 | 30.771 | 58.061 | 39.261 | 1.00 | 69.12 | AAAA | C |
| ATOM | 3510 | C | SER | 370 | 33.060 | 57.085 | 40.412 | 1.00 | 47.97 | AAAA | C |
| ATOM | 3511 | O | SER | 370 | 33.228 | 56.943 | 41.596 | 1.00 | 41.93 | AAAA | O |
| ATOM | 3512 | H | PHE | 371 | 32.967 | 55.936 | 39.792 | 1.00 | 45.48 | AAAA | H |
| ATOM | 3514 | CA | PHE | 371 | 33.223 | 54.643 | 40.356 | 1.00 | 46.29 | AAAA | C |
| ATOM | 3515 | CB | PHE | 371 | 32.952 | 53.596 | 39.287 | 1.00 | 43.53 | AAAA | C |
| ATOM | 3516 | CG | PHE | 371 | 33.724 | 53.629 | 38.012 | 1.00 | 56.45 | AAAA | C |
| ATOM | 3517 | CD1 | PHE | 371 | 34.805 | 52.807 | 37.764 | 1.00 | 58.95 | AAAA | C |
| ATOM | 3518 | CD2 | PHE | 371 | 33.371 | 54.515 | 37.004 | 1.00 | 53.92 | AAAA | C |
| ATOM | 3519 | CE1 | PHE | 371 | 35.498 | 52.842 | 36.570 | 1.00 | 59.50 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|--------|
| ATOH | 3520 | CEU | PHE | 371 | 34.048 | 54.546 | 35.817 | 1.00 | 56.49 | |
| ATOH | 3521 | CE | PHE | 371 | 35.119 | 53.716 | 35.579 | 1.00 | 56.39 | AAAA C |
| ATOH | 3522 | C | PHE | 371 | 34.654 | 54.467 | 40.895 | 1.00 | 54.84 | AAAA C |
| ATOH | 3523 | O | PHE | 371 | 35.005 | 53.592 | 41.728 | 1.00 | 52.23 | AAAA C |
| ATOH | 3524 | H | LEU | 372 | 35.633 | 55.305 | 40.510 | 1.00 | 50.17 | AAAA O |
| ATOH | 3526 | CA | LEU | 372 | 36.928 | 55.395 | 41.109 | 1.00 | 46.25 | AAAA H |
| ATOH | 3527 | CB | LEU | 372 | 38.171 | 55.812 | 40.276 | 1.00 | 44.82 | AAAA C |
| ATOH | 3528 | CG | LEU | 372 | 38.411 | 54.800 | 39.114 | 1.00 | 36.78 | AAAA C |
| ATOH | 3529 | CD1 | LEU | 372 | 38.853 | 55.643 | 37.934 | 1.00 | 45.04 | AAAA C |
| ATOH | 3530 | CD2 | LEU | 372 | 39.260 | 53.657 | 39.565 | 1.00 | 35.55 | AAAA C |
| ATOH | 3531 | C | LEU | 372 | 36.715 | 56.392 | 42.243 | 1.00 | 42.26 | AAAA C |
| ATOH | 3532 | O | LEU | 372 | 37.224 | 57.507 | 42.364 | 1.00 | 38.37 | AAAA C |
| ATOH | 3533 | H | LYS | 373 | 35.970 | 55.862 | 43.192 | 1.00 | 47.06 | AAAA O |
| ATOH | 3535 | CA | LYS | 373 | 35.527 | 56.509 | 44.415 | 1.00 | 50.19 | AAAA N |
| ATOH | 3536 | CB | LYS | 373 | 34.546 | 55.521 | 45.077 | 1.00 | 56.74 | AAAA C |
| ATOH | 3537 | CG | LYS | 373 | 33.645 | 56.162 | 46.119 | 1.00 | 59.64 | AAAA C |
| ATOH | 3538 | CD | LYS | 373 | 32.529 | 56.955 | 45.441 | 0.01 | 60.17 | AAAA C |
| ATOH | 3539 | CE | LYS | 373 | 31.674 | 57.687 | 46.460 | 0.01 | 60.45 | AAAA C |
| ATOH | 3540 | HC | LYS | 373 | 31.083 | 58.933 | 45.899 | 0.01 | 60.38 | AAAA C |
| ATOH | 3544 | C | LYS | 373 | 36.646 | 56.863 | 45.366 | 1.00 | 49.72 | AAAA N |
| ATOH | 3545 | O | LYS | 373 | 36.636 | 57.960 | 45.907 | 1.00 | 42.42 | AAAA C |
| ATOH | 3546 | H | ASN | 374 | 37.657 | 55.986 | 45.513 | 1.00 | 54.43 | AAAA O |
| ATOH | 3549 | CA | ASN | 374 | 38.765 | 56.352 | 46.410 | 1.00 | 59.92 | AAAA N |
| ATOH | 3549 | CB | ASN | 374 | 39.080 | 55.154 | 47.314 | 1.00 | 63.16 | AAAA C |
| ATOH | 3550 | CG | ASN | 374 | 38.009 | 54.978 | 48.396 | 1.00 | 64.53 | AAAA C |
| ATOH | 3551 | OD1 | ASN | 374 | 37.892 | 53.972 | 49.096 | 1.00 | 66.40 | AAAA C |
| ATOH | 3552 | HD2 | ASN | 374 | 37.160 | 55.965 | 48.578 | 1.00 | 52.88 | AAAA O |
| ATOH | 3555 | C | ASN | 374 | 40.043 | 56.892 | 45.786 | 1.00 | 62.35 | AAAA N |
| ATOH | 3556 | O | ASN | 374 | 41.031 | 57.223 | 46.479 | 1.00 | 63.08 | AAAA C |
| ATOH | 3557 | H | LEU | 375 | 40.091 | 56.893 | 44.438 | 1.00 | 58.34 | AAAA O |
| ATOH | 3559 | CA | LEU | 375 | 41.305 | 57.374 | 43.795 | 1.00 | 54.73 | AAAA N |
| ATOH | 3560 | CB | LEU | 375 | 41.099 | 57.359 | 42.288 | 1.00 | 56.41 | AAAA C |
| ATOH | 3561 | CG | LEU | 375 | 42.396 | 57.422 | 41.459 | 1.00 | 54.12 | AAAA C |
| ATOH | 3562 | CD1 | LEU | 375 | 43.135 | 56.112 | 41.689 | 1.00 | 37.88 | AAAA C |
| ATOH | 3563 | CD2 | LEU | 375 | 42.030 | 57.796 | 40.041 | 1.00 | 40.97 | AAAA C |
| ATOH | 3564 | C | LEU | 375 | 41.712 | 59.754 | 44.245 | 1.00 | 52.37 | AAAA C |
| ATOH | 3565 | O | LEU | 375 | 41.151 | 59.777 | 43.877 | 1.00 | 50.11 | AAAA O |
| ATOH | 3566 | H | ARG | 376 | 42.801 | 59.874 | 44.982 | 1.00 | 55.16 | AAAA C |
| ATOH | 3569 | CA | ARG | 376 | 43.320 | 60.155 | 45.434 | 1.00 | 55.45 | AAAA H |
| ATOH | 3569 | CB | ARG | 376 | 43.706 | 60.222 | 46.929 | 1.00 | 52.63 | AAAA C |
| ATOH | 3571 | CG | ARG | 376 | 44.288 | 59.907 | 47.415 | 1.00 | 69.10 | AAAA C |
| ATOH | 3571 | CD | ARG | 376 | 44.286 | 59.917 | 48.944 | 1.00 | 81.17 | AAAA C |
| ATOH | 3572 | HE | ARG | 376 | 45.377 | 57.926 | 49.410 | 1.00 | 84.46 | AAAA C |
| ATOH | 3574 | CD | ARG | 376 | 46.619 | 58.380 | 49.598 | 1.00 | 85.64 | AAAA H |
| ATOH | 3575 | HH1 | ARG | 376 | 46.966 | 59.645 | 49.383 | 1.00 | 81.84 | AAAA C |
| ATOH | 3575 | HH2 | ARG | 376 | 47.571 | 57.548 | 50.012 | 1.00 | 94.15 | AAAA H |
| ATOH | 3581 | C | ARG | 376 | 44.556 | 60.544 | 44.633 | 1.00 | 50.16 | AAAA C |
| ATOH | 3582 | O | ARG | 376 | 44.746 | 61.728 | 44.465 | 1.00 | 44.25 | AAAA C |
| ATOH | 3582 | H | LEU | 377 | 45.375 | 59.578 | 44.219 | 1.00 | 50.99 | AAAA O |
| ATOH | 3588 | CA | LEU | 377 | 46.526 | 59.942 | 43.379 | 1.00 | 49.40 | AAAA H |
| ATOH | 3588 | CB | LEU | 377 | 47.596 | 60.411 | 44.329 | 1.00 | 64.72 | AAAA C |
| ATOH | 3587 | CG | LEU | 377 | 49.806 | 59.577 | 44.667 | 1.00 | 70.76 | AAAA C |
| ATOH | 3588 | CD1 | LEU | 377 | 50.031 | 60.157 | 43.954 | 1.00 | 63.32 | AAAA C |
| ATOH | 3589 | CD2 | LEU | 377 | 49.010 | 59.696 | 46.179 | 1.00 | 68.60 | AAAA C |
| ATOH | 3590 | C | LEU | 377 | 47.043 | 59.022 | 42.311 | 1.00 | 46.33 | AAAA C |
| ATOH | 3591 | O | LEU | 377 | 46.868 | 57.788 | 42.286 | 1.00 | 45.17 | AAAA O |
| ATOH | 3592 | H | ILE | 378 | 47.448 | 59.675 | 41.199 | 1.00 | 45.12 | AAAA C |
| ATOH | 3594 | CA | ILE | 378 | 48.042 | 58.976 | 40.042 | 1.00 | 49.10 | AAAA N |
| ATOH | 3595 | CB | ILE | 378 | 47.342 | 59.303 | 39.724 | 1.00 | 46.36 | AAAA C |
| ATOH | 3596 | CG2 | ILE | 378 | 48.115 | 58.696 | 37.574 | 1.00 | 34.36 | AAAA C |
| ATOH | 3597 | CG1 | ILE | 378 | 45.971 | 58.862 | 38.829 | 1.00 | 38.59 | AAAA C |
| ATOH | 3598 | CD1 | ILE | 378 | 44.999 | 59.515 | 37.765 | 1.00 | 37.19 | AAAA C |
| ATOH | 3599 | C | ILE | 378 | 49.524 | 59.381 | 40.003 | 1.00 | 49.87 | AAAA C |
| ATOH | 3600 | O | ILE | 378 | 49.801 | 60.595 | 40.040 | 1.00 | 44.72 | AAAA C |
| ATOH | 3601 | H | LEU | 379 | 50.454 | 58.423 | 40.067 | 1.00 | 49.97 | AAAA O |
| ATOH | 3603 | CA | LEU | 379 | 51.866 | 59.712 | 40.344 | 1.00 | 48.49 | AAAA H |
| ATOH | 3604 | CB | LEU | 379 | 52.575 | 57.531 | 41.054 | 1.00 | 48.44 | AAAA C |
| ATOH | 3605 | CG | LEU | 379 | 52.234 | 57.363 | 42.554 | 1.00 | 50.29 | AAAA C |
| ATOH | 3606 | CD1 | LEU | 379 | 52.926 | 56.187 | 43.217 | 1.00 | 39.59 | AAAA C |
| ATOH | 3607 | CD2 | LEU | 379 | 52.616 | 58.625 | 43.300 | 1.00 | 42.89 | AAAA C |
| ATOH | 3608 | C | LEU | 379 | 52.609 | 59.019 | 39.080 | 1.00 | 50.94 | AAAA C |
| ATOH | 3609 | O | LEU | 379 | 53.576 | 59.788 | 39.139 | 1.00 | 54.23 | AAAA C |
| ATOH | 3610 | H | GLY | 380 | 52.175 | 58.423 | 37.972 | 1.00 | 49.67 | AAAA O |
| ATOH | 3612 | CA | GLY | 380 | 52.831 | 58.715 | 36.702 | 1.00 | 49.94 | AAAA H |
| ATOH | 3613 | C | GLY | 380 | 54.249 | 58.155 | 36.624 | 1.00 | 52.70 | AAAA C |
| ATOH | 3614 | O | GLY | 380 | 55.026 | 58.657 | 35.803 | 1.00 | 49.94 | AAAA C |
| ATOH | 3615 | H | GLU | 381 | 54.549 | 57.033 | 37.272 | 1.00 | 52.51 | AAAA O |
| ATOH | 3617 | CA | GLU | 381 | 55.849 | 56.386 | 37.243 | 1.00 | 52.33 | AAAA N |
| ATOH | 3618 | CB | GLU | 381 | 56.055 | 55.310 | 38.323 | 1.00 | 45.22 | AAAA C |
| ATOH | 3619 | CG | GLU | 381 | 55.402 | 55.779 | 39.636 | 1.00 | 52.91 | AAAA C |
| ATOH | 3620 | CD | GLU | 381 | 56.050 | 55.192 | 40.873 | 1.00 | 42.11 | AAAA C |
| ATOH | 3621 | OE1 | GLU | 381 | 56.160 | 53.966 | 40.890 | 1.00 | 40.26 | AAAA C |
| ATOH | 3622 | OE2 | GLU | 381 | 56.379 | 56.014 | 41.754 | 1.00 | 51.32 | AAAA O |
| ATOH | 3623 | C | GLU | 381 | 56.078 | 55.784 | 35.858 | 1.00 | 55.86 | AAAA C |
| ATOH | 3624 | O | GLU | 381 | 57.216 | 55.652 | 35.345 | 1.00 | 54.61 | AAAA C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 3625 | H | GLU | 382 | 54.980 | 55.449 | 35.157 | 1.00 | 53.56 | AAAA | N |
| ATOM | 3627 | CA | GLU | 382 | 55.091 | 55.018 | 33.766 | 1.00 | 48.15 | AAAA | C |
| ATOM | 3628 | CB | GLU | 382 | 55.051 | 53.550 | 33.532 | 1.00 | 35.27 | AAAA | C |
| ATOM | 3629 | CG | GLU | 382 | 54.739 | 53.225 | 32.051 | 1.00 | 49.69 | AAAA | C |
| ATOM | 3630 | CD | GLU | 382 | 54.676 | 51.719 | 31.807 | 1.00 | 56.45 | AAAA | C |
| ATOM | 3631 | OE1 | GLU | 382 | 55.062 | 50.924 | 32.705 | 1.00 | 61.66 | AAAA | O |
| ATOM | 3632 | OE2 | GLU | 382 | 54.264 | 51.201 | 30.745 | 1.00 | 57.69 | AAAA | O |
| ATOM | 3633 | C | GLU | 382 | 54.006 | 55.732 | 32.973 | 1.00 | 50.84 | AAAA | C |
| ATOM | 3634 | O | GLU | 382 | 53.097 | 56.282 | 33.598 | 1.00 | 49.44 | AAAA | O |
| ATOM | 3635 | H | GLN | 383 | 54.347 | 56.256 | 31.780 | 1.00 | 52.25 | AAAA | H |
| ATOM | 3637 | CA | GLN | 383 | 53.498 | 57.153 | 31.016 | 1.00 | 40.15 | AAAA | C |
| ATOM | 3638 | CB | GLN | 383 | 53.914 | 58.609 | 31.155 | 1.00 | 28.50 | AAAA | C |
| ATOM | 3639 | CG | GLN | 383 | 54.489 | 58.909 | 32.542 | 1.00 | 31.10 | AAAA | C |
| ATOM | 3640 | CD | GLN | 383 | 54.950 | 60.301 | 32.752 | 1.00 | 33.19 | AAAA | C |
| ATOM | 3641 | OE1 | GLN | 383 | 55.186 | 60.840 | 31.683 | 1.00 | 40.34 | AAAA | O |
| ATOM | 3642 | OE2 | GLN | 383 | 55.043 | 60.943 | 33.934 | 1.00 | 36.30 | AAAA | H |
| ATOM | 3645 | C | GLN | 383 | 53.426 | 56.744 | 29.563 | 1.00 | 40.45 | AAAA | C |
| ATOM | 3646 | O | GLN | 383 | 54.131 | 55.858 | 29.139 | 1.00 | 43.45 | AAAA | O |
| ATOM | 3647 | H | LEU | 384 | 52.375 | 57.195 | 28.860 | 1.00 | 42.54 | AAAA | H |
| ATOM | 3649 | CA | LEU | 384 | 52.257 | 56.889 | 27.443 | 1.00 | 43.24 | AAAA | C |
| ATOM | 3650 | CB | LEU | 384 | 50.814 | 57.011 | 26.949 | 1.00 | 43.79 | AAAA | C |
| ATOM | 3651 | CG | LEU | 384 | 49.818 | 56.235 | 27.861 | 1.00 | 41.21 | AAAA | C |
| ATOM | 3652 | CD1 | LEU | 384 | 48.611 | 57.095 | 28.221 | 1.00 | 33.99 | AAAA | C |
| ATOM | 3653 | CD2 | LEU | 384 | 49.405 | 54.968 | 27.149 | 1.00 | 33.20 | AAAA | C |
| ATOM | 3654 | C | LEU | 384 | 53.204 | 57.809 | 26.672 | 1.00 | 40.51 | AAAA | C |
| ATOM | 3655 | O | LEU | 384 | 53.582 | 58.872 | 27.177 | 1.00 | 29.66 | AAAA | O |
| ATOM | 3656 | H | GLU | 385 | 53.659 | 57.319 | 25.531 | 1.00 | 45.22 | AAAA | N |
| ATOM | 3658 | CA | GLU | 385 | 54.410 | 58.116 | 24.570 | 1.00 | 49.98 | AAAA | C |
| ATOM | 3659 | CB | GLU | 385 | 54.424 | 57.475 | 23.174 | 1.00 | 60.50 | AAAA | C |
| ATOM | 3660 | CG | GLU | 385 | 55.045 | 56.095 | 23.106 | 1.00 | 68.76 | AAAA | C |
| ATOM | 3661 | CD | GLU | 385 | 54.195 | 54.951 | 23.592 | 1.00 | 72.07 | AAAA | C |
| ATOM | 3662 | OE1 | GLU | 385 | 53.150 | 55.213 | 24.244 | 1.00 | 81.88 | AAAA | O |
| ATOM | 3663 | OE2 | GLU | 385 | 54.565 | 53.786 | 23.301 | 1.00 | 73.13 | AAAA | O |
| ATOM | 3664 | C | GLU | 385 | 53.829 | 59.515 | 24.450 | 1.00 | 47.41 | AAAA | C |
| ATOM | 3665 | O | GLU | 385 | 52.635 | 59.706 | 24.184 | 1.00 | 54.43 | AAAA | O |
| ATOM | 3666 | H | GLY | 386 | 54.614 | 60.470 | 24.902 | 1.00 | 43.69 | AAAA | H |
| ATOM | 3669 | CA | GLY | 386 | 54.191 | 61.870 | 24.897 | 1.00 | 40.34 | AAAA | C |
| ATOM | 3669 | C | GLY | 386 | 54.286 | 62.449 | 26.309 | 1.00 | 40.65 | AAAA | C |
| ATOM | 3670 | O | GLY | 386 | 53.930 | 63.615 | 26.491 | 1.00 | 39.75 | AAAA | O |
| ATOM | 3671 | H | ASN | 387 | 54.441 | 61.537 | 27.272 | 1.00 | 40.75 | AAAA | H |
| ATOM | 3673 | CA | ASN | 387 | 54.479 | 61.912 | 28.675 | 1.00 | 49.18 | AAAA | C |
| ATOM | 3674 | CB | ASN | 387 | 55.500 | 63.094 | 28.874 | 1.00 | 44.41 | AAAA | C |
| ATOM | 3675 | CG | ASN | 387 | 56.925 | 62.541 | 28.722 | 1.00 | 61.51 | AAAA | C |
| ATOM | 3676 | CD1 | ASN | 387 | 57.199 | 61.313 | 28.677 | 1.00 | 57.85 | AAAA | O |
| ATOM | 3677 | ND2 | ASN | 387 | 58.063 | 63.251 | 28.592 | 1.00 | 61.96 | AAAA | H |
| ATOM | 3680 | C | ASN | 387 | 53.095 | 62.100 | 29.299 | 1.00 | 48.46 | AAAA | C |
| ATOM | 3681 | O | ASN | 387 | 52.636 | 62.891 | 30.218 | 1.00 | 48.99 | AAAA | O |
| ATOM | 3682 | H | TYR | 388 | 52.214 | 61.116 | 29.058 | 1.00 | 46.29 | AAAA | H |
| ATOM | 3684 | CA | TYR | 388 | 50.846 | 61.199 | 29.540 | 1.00 | 45.09 | AAAA | C |
| ATOM | 3685 | CB | TYR | 388 | 49.823 | 60.957 | 28.399 | 1.00 | 40.70 | AAAA | C |
| ATOM | 3686 | CG | TYR | 388 | 49.925 | 62.056 | 27.373 | 1.00 | 42.24 | AAAA | C |
| ATOM | 3687 | CD1 | TYR | 388 | 50.343 | 61.984 | 26.064 | 1.00 | 44.38 | AAAA | C |
| ATOM | 3689 | CE1 | TYR | 388 | 50.401 | 62.895 | 25.157 | 1.00 | 35.51 | AAAA | C |
| ATOM | 3689 | CD2 | TYR | 388 | 49.625 | 63.356 | 27.709 | 1.00 | 44.67 | AAAA | C |
| ATOM | 3690 | CE2 | TYR | 388 | 49.699 | 64.428 | 26.830 | 1.00 | 38.14 | AAAA | C |
| ATOM | 3691 | CS | TYR | 388 | 50.087 | 64.148 | 25.555 | 1.00 | 41.27 | AAAA | C |
| ATOM | 3692 | OH | TYR | 388 | 50.151 | 65.181 | 24.604 | 1.00 | 50.18 | AAAA | O |
| ATOM | 3694 | C | TYR | 388 | 50.563 | 60.288 | 30.714 | 1.00 | 41.88 | AAAA | C |
| ATOM | 3695 | O | TYR | 388 | 50.727 | 59.092 | 30.511 | 1.00 | 32.99 | AAAA | O |
| ATOM | 3696 | H | SER | 389 | 50.020 | 60.917 | 31.763 | 1.00 | 45.42 | AAAA | H |
| ATOM | 3698 | CA | SER | 389 | 49.591 | 60.131 | 32.931 | 1.00 | 50.13 | AAAA | C |
| ATOM | 3699 | CB | SER | 389 | 49.798 | 60.894 | 34.261 | 1.00 | 45.57 | AAAA | C |
| ATOM | 3700 | CG | SER | 389 | 51.185 | 60.899 | 34.504 | 1.00 | 51.11 | AAAA | O |
| ATOM | 3702 | C | SER | 389 | 48.097 | 59.813 | 32.804 | 1.00 | 48.11 | AAAA | C |
| ATOM | 3703 | O | SER | 389 | 47.686 | 58.792 | 33.336 | 1.00 | 49.25 | AAAA | O |
| ATOM | 3704 | H | PHE | 390 | 47.321 | 60.685 | 32.196 | 1.00 | 42.56 | AAAA | H |
| ATOM | 3706 | CA | PHE | 390 | 45.867 | 60.595 | 32.146 | 1.00 | 40.76 | AAAA | C |
| ATOM | 3707 | CB | PHE | 390 | 45.241 | 61.581 | 33.139 | 1.00 | 44.80 | AAAA | C |
| ATOM | 3708 | CG | PHE | 390 | 43.764 | 61.358 | 33.328 | 1.00 | 40.53 | AAAA | C |
| ATOM | 3709 | CD1 | PHE | 390 | 43.406 | 60.273 | 34.089 | 1.00 | 40.80 | AAAA | C |
| ATOM | 3710 | CD2 | PHE | 390 | 42.768 | 62.157 | 32.748 | 1.00 | 35.59 | AAAA | C |
| ATOM | 3711 | CE1 | PHE | 390 | 42.050 | 59.985 | 34.312 | 1.00 | 47.09 | AAAA | C |
| ATOM | 3712 | CE2 | PHE | 390 | 41.454 | 61.824 | 32.965 | 1.00 | 44.50 | AAAA | C |
| ATOM | 3713 | CC | PHE | 390 | 41.063 | 60.745 | 33.739 | 1.00 | 34.54 | AAAA | C |
| ATOM | 3714 | C | PHE | 390 | 45.372 | 60.929 | 30.720 | 1.00 | 38.54 | AAAA | C |
| ATOM | 3715 | O | PHE | 390 | 45.542 | 61.918 | 30.126 | 1.00 | 40.29 | AAAA | O |
| ATOM | 3716 | H | TYR | 391 | 44.819 | 59.818 | 30.096 | 1.00 | 33.48 | AAAA | H |
| ATOM | 3719 | CA | TYR | 391 | 44.596 | 59.782 | 28.663 | 1.00 | 38.58 | AAAA | C |
| ATOM | 3719 | CB | TYR | 391 | 45.579 | 58.871 | 27.972 | 1.00 | 38.95 | AAAA | C |
| ATOM | 3720 | CG | TYR | 391 | 45.760 | 59.006 | 26.503 | 1.00 | 44.54 | AAAA | C |
| ATOM | 3721 | CD1 | TYR | 391 | 46.822 | 59.815 | 26.052 | 1.00 | 47.14 | AAAA | C |
| ATOM | 3722 | CE1 | TYR | 391 | 47.057 | 59.993 | 24.722 | 1.00 | 46.03 | AAAA | C |
| ATOM | 3723 | CD2 | TYR | 391 | 44.927 | 58.390 | 25.584 | 1.00 | 46.94 | AAAA | C |
| ATOM | 3724 | CE2 | TYR | 391 | 45.157 | 58.560 | 24.242 | 1.00 | 47.45 | AAAA | C |
| ATOM | 3725 | CC | TYR | 391 | 46.207 | 59.350 | 23.830 | 1.00 | 45.84 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 3726 | OH | TTR | 391 | 46.374 | 59.492 | 22.481 | 1.00 | 44.70 | AAAA | O |
| ATOH | 3728 | C | TTR | 391 | 43.194 | 59.232 | 28.349 | 1.00 | 39.74 | AAAA | C |
| ATOH | 3729 | O | TTR | 391 | 42.841 | 58.103 | 28.730 | 1.00 | 38.49 | AAAA | O |
| ATOH | 3730 | H | VAL | 392 | 42.417 | 60.158 | 27.779 | 1.00 | 37.07 | AAAA | N |
| ATOH | 3732 | CA | VAL | 392 | 40.958 | 59.874 | 27.603 | 1.00 | 39.52 | AAAA | C |
| ATOH | 3733 | CB | VAL | 392 | 40.075 | 60.880 | 28.440 | 1.00 | 41.12 | AAAA | C |
| ATOH | 3734 | CG1 | VAL | 392 | 38.612 | 60.464 | 28.472 | 1.00 | 37.96 | AAAA | C |
| ATOH | 3735 | CG2 | VAL | 392 | 40.666 | 61.041 | 29.841 | 1.00 | 33.19 | AAAA | C |
| ATOH | 3736 | C | VAL | 392 | 40.531 | 60.092 | 26.182 | 1.00 | 31.08 | AAAA | C |
| ATOH | 3737 | O | VAL | 392 | 40.508 | 61.277 | 25.804 | 1.00 | 34.71 | AAAA | O |
| ATOH | 3738 | H | LEU | 393 | 40.299 | 59.113 | 25.383 | 1.00 | 34.62 | AAAA | H |
| ATOH | 3740 | CA | LEU | 393 | 39.948 | 59.259 | 23.977 | 1.00 | 38.12 | AAAA | C |
| ATOH | 3741 | CB | LEU | 393 | 41.200 | 59.036 | 23.096 | 1.00 | 42.49 | AAAA | C |
| ATOH | 3742 | CG | LEU | 393 | 41.023 | 58.649 | 21.586 | 1.00 | 26.48 | AAAA | C |
| ATOH | 3743 | CD1 | LEU | 393 | 41.129 | 59.879 | 20.753 | 1.00 | 26.57 | AAAA | C |
| ATOH | 3744 | CD2 | LEU | 393 | 42.078 | 57.589 | 21.244 | 1.00 | 29.98 | AAAA | C |
| ATOH | 3745 | C | LEU | 393 | 38.821 | 58.375 | 23.482 | 1.00 | 39.15 | AAAA | C |
| ATOH | 3746 | O | LEU | 393 | 38.760 | 57.173 | 23.799 | 1.00 | 37.90 | AAAA | O |
| ATOH | 3747 | H | ASP | 394 | 38.015 | 58.973 | 22.565 | 1.00 | 43.38 | AAAA | N |
| ATOH | 3749 | CA | ASP | 394 | 36.888 | 58.215 | 21.975 | 1.00 | 44.77 | AAAA | C |
| ATOH | 3750 | CB | ASP | 394 | 37.445 | 57.073 | 21.120 | 1.00 | 44.80 | AAAA | C |
| ATOH | 3751 | CG | ASP | 394 | 36.466 | 56.477 | 20.156 | 1.00 | 47.14 | AAAA | C |
| ATOH | 3752 | OD1 | ASP | 394 | 36.750 | 55.577 | 19.333 | 1.00 | 52.81 | AAAA | O |
| ATOH | 3753 | OD2 | ASP | 394 | 35.311 | 56.948 | 20.180 | 1.00 | 49.27 | AAAA | O |
| ATOH | 3754 | C | ASP | 394 | 35.936 | 57.619 | 23.021 | 1.00 | 43.17 | AAAA | C |
| ATOH | 3755 | O | ASP | 394 | 35.831 | 56.385 | 23.212 | 1.00 | 43.51 | AAAA | O |
| ATOH | 3756 | H | ASH | 395 | 35.299 | 58.495 | 23.746 | 1.00 | 39.90 | AAAA | H |
| ATOH | 3758 | CA | ASH | 395 | 34.305 | 58.158 | 24.776 | 1.00 | 46.32 | AAAA | C |
| ATOH | 3759 | CB | ASH | 395 | 34.804 | 58.512 | 26.212 | 1.00 | 42.96 | AAAA | C |
| ATOH | 3760 | CG | ASH | 395 | 35.992 | 57.619 | 26.579 | 1.00 | 36.92 | AAAA | C |
| ATOH | 3761 | OD1 | ASH | 395 | 36.013 | 56.394 | 26.796 | 1.00 | 21.65 | AAAA | O |
| ATOH | 3762 | OD2 | ASH | 395 | 37.075 | 58.409 | 26.558 | 1.00 | 27.87 | AAAA | H |
| ATOH | 3765 | C | ASH | 395 | 32.932 | 58.816 | 24.541 | 1.00 | 40.44 | AAAA | C |
| ATOH | 3766 | O | ASH | 395 | 32.749 | 59.992 | 24.882 | 1.00 | 37.06 | AAAA | O |
| ATOH | 3767 | H | GLN | 396 | 32.073 | 58.055 | 23.877 | 1.00 | 46.74 | AAAA | H |
| ATOH | 3769 | CA | GLN | 396 | 30.771 | 58.582 | 23.421 | 1.00 | 52.93 | AAAA | C |
| ATOH | 3770 | CB | GLN | 396 | 29.849 | 57.567 | 22.744 | 1.00 | 52.29 | AAAA | C |
| ATOH | 3771 | CG | GLN | 396 | 30.173 | 57.405 | 21.257 | 1.00 | 46.42 | AAAA | C |
| ATOH | 3772 | CD | GLN | 396 | 29.917 | 55.991 | 20.840 | 1.00 | 55.21 | AAAA | C |
| ATOH | 3773 | OE1 | GLN | 396 | 28.835 | 55.421 | 21.312 | 1.00 | 61.17 | AAAA | O |
| ATOH | 3774 | NE2 | GLN | 396 | 30.628 | 55.411 | 19.971 | 1.00 | 55.79 | AAAA | H |
| ATOH | 3777 | C | GLN | 396 | 29.974 | 59.224 | 24.458 | 1.00 | 49.64 | AAAA | C |
| ATOH | 3778 | O | GLN | 396 | 29.407 | 60.267 | 24.113 | 1.00 | 51.63 | AAAA | O |
| ATOH | 3779 | H | ASH | 397 | 29.717 | 58.681 | 25.633 | 1.00 | 49.95 | AAAA | H |
| ATOH | 3781 | CA | ASH | 397 | 28.783 | 59.196 | 26.632 | 1.00 | 51.72 | AAAA | C |
| ATOH | 3782 | CB | ASH | 397 | 27.969 | 57.959 | 27.093 | 1.00 | 35.94 | AAAA | C |
| ATOH | 3783 | CG | ASH | 397 | 27.231 | 57.430 | 25.860 | 1.00 | 49.09 | AAAA | C |
| ATOH | 3784 | CD1 | ASH | 397 | 26.591 | 58.304 | 25.229 | 1.00 | 49.32 | AAAA | O |
| ATOH | 3785 | OD | ASH | 397 | 27.259 | 56.175 | 25.431 | 1.00 | 43.31 | AAAA | H |
| ATOH | 3788 | C | ASH | 397 | 29.367 | 59.945 | 27.800 | 1.00 | 52.98 | AAAA | C |
| ATOH | 3789 | O | ASH | 397 | 28.586 | 60.344 | 29.627 | 1.00 | 53.33 | AAAA | O |
| ATOH | 3790 | H | LEU | 399 | 30.682 | 59.990 | 29.001 | 1.00 | 55.73 | AAAA | H |
| ATOH | 3792 | CA | LEU | 399 | 31.312 | 60.550 | 29.179 | 1.00 | 52.12 | AAAA | C |
| ATOH | 3793 | CB | LEU | 399 | 32.827 | 60.388 | 29.148 | 1.00 | 48.47 | AAAA | C |
| ATOH | 3794 | CG | LEU | 399 | 33.606 | 60.283 | 30.460 | 1.00 | 41.81 | AAAA | C |
| ATOH | 3795 | CD1 | LEU | 399 | 33.417 | 58.939 | 31.136 | 1.00 | 40.35 | AAAA | C |
| ATOH | 3796 | CD2 | LEU | 399 | 35.070 | 60.608 | 30.082 | 1.00 | 39.03 | AAAA | C |
| ATOH | 3797 | C | LEU | 399 | 30.923 | 61.995 | 29.353 | 1.00 | 52.35 | AAAA | C |
| ATOH | 3798 | O | LEU | 399 | 31.422 | 62.909 | 28.681 | 1.00 | 49.91 | AAAA | O |
| ATOH | 3799 | H | GLN | 399 | 30.241 | 62.225 | 30.469 | 1.00 | 58.76 | AAAA | N |
| ATOH | 3801 | CA | GLN | 399 | 29.688 | 63.558 | 30.796 | 1.00 | 60.03 | AAAA | C |
| ATOH | 3802 | CB | GLN | 399 | 28.236 | 63.331 | 31.262 | 1.00 | 59.55 | AAAA | C |
| ATOH | 3803 | CG | GLN | 399 | 27.235 | 63.962 | 30.316 | 1.00 | 73.07 | AAAA | C |
| ATOH | 3804 | CD | GLN | 399 | 25.944 | 63.146 | 30.340 | 1.00 | 78.39 | AAAA | C |
| ATOH | 3805 | OE1 | GLN | 399 | 25.097 | 63.455 | 31.194 | 1.00 | 71.79 | AAAA | O |
| ATOH | 3806 | NE2 | GLN | 399 | 25.856 | 62.158 | 29.440 | 1.00 | 69.88 | AAAA | H |
| ATOH | 3809 | C | GLN | 399 | 30.490 | 64.252 | 31.888 | 1.00 | 54.49 | AAAA | C |
| ATOH | 3810 | O | GLN | 399 | 30.528 | 65.477 | 32.068 | 1.00 | 51.96 | AAAA | O |
| ATOH | 3811 | H | GLN | 400 | 31.058 | 63.389 | 32.734 | 1.00 | 50.44 | AAAA | H |
| ATOH | 3813 | CA | GLN | 400 | 31.938 | 63.948 | 33.756 | 1.00 | 53.83 | AAAA | C |
| ATOH | 3814 | CB | GLN | 400 | 31.215 | 64.314 | 35.049 | 1.00 | 51.97 | AAAA | C |
| ATOH | 3815 | CG | GLN | 400 | 30.717 | 63.150 | 35.887 | 1.00 | 58.99 | AAAA | C |
| ATOH | 3816 | CD | GLN | 400 | 30.678 | 63.430 | 37.389 | 1.00 | 65.82 | AAAA | C |
| ATOH | 3817 | OE1 | GLN | 400 | 30.906 | 64.502 | 37.962 | 1.00 | 68.10 | AAAA | O |
| ATOH | 3818 | NE2 | GLN | 400 | 30.341 | 62.444 | 38.222 | 1.00 | 55.35 | AAAA | H |
| ATOH | 3821 | C | GLN | 400 | 33.113 | 63.008 | 34.052 | 1.00 | 52.08 | AAAA | C |
| ATOH | 3822 | O | GLN | 400 | 33.107 | 61.783 | 33.942 | 1.00 | 51.90 | AAAA | O |
| ATOH | 3823 | H | LEU | 401 | 34.073 | 63.580 | 34.751 | 1.00 | 49.58 | AAAA | N |
| ATOH | 3825 | CA | LEU | 401 | 35.175 | 62.844 | 35.334 | 1.00 | 49.57 | AAAA | C |
| ATOH | 3826 | CB | LEU | 401 | 36.378 | 63.803 | 35.260 | 1.00 | 47.94 | AAAA | C |
| ATOH | 3827 | CG | LEU | 401 | 36.638 | 64.237 | 33.772 | 1.00 | 46.61 | AAAA | C |
| ATOH | 3828 | CD1 | LEU | 401 | 37.658 | 65.326 | 33.677 | 1.00 | 39.09 | AAAA | C |
| ATOH | 3829 | CD2 | LEU | 401 | 36.919 | 63.069 | 32.860 | 1.00 | 40.72 | AAAA | C |
| ATOH | 3830 | C | LEU | 401 | 34.866 | 62.357 | 36.734 | 1.00 | 51.23 | AAAA | C |
| ATOH | 3831 | O | LEU | 401 | 34.258 | 61.299 | 36.892 | 1.00 | 49.06 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 3832 | H | TRP | 402 | 35.297 | 63.140 | 37.690 | 1.00 | 54.58 | AAAA | H |
| ATOM | 3834 | CA | TRP | 402 | 34.975 | 63.090 | 39.097 | 1.00 | 59.76 | AAAA | C |
| ATOM | 3835 | CB | TRP | 402 | 36.279 | 62.953 | 39.933 | 1.00 | 59.56 | AAAA | C |
| ATOM | 3836 | CG | TRP | 402 | 36.971 | 61.624 | 39.737 | 1.00 | 58.17 | AAAA | C |
| ATOM | 3837 | CD2 | TRP | 402 | 37.981 | 61.243 | 38.784 | 1.00 | 53.18 | AAAA | C |
| ATOM | 3838 | CE2 | TRP | 402 | 38.286 | 59.897 | 39.002 | 1.00 | 56.61 | AAAA | C |
| ATOM | 3839 | CE3 | TRP | 402 | 38.643 | 61.917 | 37.764 | 1.00 | 43.25 | AAAA | C |
| ATOM | 3840 | CD1 | TRP | 402 | 36.719 | 60.517 | 40.459 | 1.00 | 53.50 | AAAA | C |
| ATOM | 3841 | HE1 | TRP | 402 | 37.488 | 59.467 | 40.032 | 1.00 | 57.66 | AAAA | H |
| ATOM | 3843 | CZ2 | TRP | 402 | 39.212 | 59.160 | 38.249 | 1.00 | 51.44 | AAAA | C |
| ATOM | 3844 | CZ3 | TRP | 402 | 39.546 | 61.199 | 37.026 | 1.00 | 53.69 | AAAA | C |
| ATOM | 3845 | CH2 | TRP | 402 | 39.820 | 59.857 | 37.263 | 1.00 | 50.75 | AAAA | C |
| ATOM | 3846 | C | TRP | 402 | 34.223 | 64.389 | 39.429 | 1.00 | 64.09 | AAAA | C |
| ATOM | 3847 | O | TRP | 402 | 34.408 | 65.449 | 38.808 | 1.00 | 61.98 | AAAA | O |
| ATOM | 3848 | H | ASP | 403 | 33.503 | 64.418 | 40.551 | 1.00 | 68.85 | AAAA | H |
| ATOM | 3850 | CA | ASP | 403 | 32.947 | 65.668 | 41.068 | 1.00 | 67.83 | AAAA | C |
| ATOM | 3851 | CB | ASP | 403 | 31.918 | 65.343 | 42.151 | 1.00 | 72.19 | AAAA | C |
| ATOM | 3852 | CG | ASP | 403 | 30.853 | 66.417 | 42.306 | 1.00 | 73.08 | AAAA | C |
| ATOM | 3853 | OD1 | ASP | 403 | 31.177 | 67.625 | 42.297 | 1.00 | 71.67 | AAAA | O |
| ATOM | 3854 | OD2 | ASP | 403 | 29.693 | 65.979 | 42.454 | 1.00 | 75.08 | AAAA | O |
| ATOM | 3855 | C | ASP | 403 | 34.005 | 66.607 | 41.607 | 1.00 | 66.63 | AAAA | C |
| ATOM | 3856 | O | ASP | 403 | 34.245 | 66.672 | 42.811 | 1.00 | 67.18 | AAAA | O |
| ATOM | 3857 | H | TRP | 404 | 34.449 | 67.588 | 40.846 | 1.00 | 69.29 | AAAA | H |
| ATOM | 3859 | CA | TRP | 404 | 35.412 | 68.588 | 41.291 | 1.00 | 77.11 | AAAA | C |
| ATOM | 3860 | CB | TRP | 404 | 35.859 | 69.409 | 40.063 | 1.00 | 79.10 | AAAA | C |
| ATOM | 3861 | CG | TRP | 404 | 36.504 | 68.509 | 39.047 | 1.00 | 82.59 | AAAA | C |
| ATOM | 3862 | CD2 | TRP | 404 | 37.294 | 67.346 | 39.322 | 1.00 | 84.82 | AAAA | C |
| ATOM | 3863 | CE2 | TRP | 404 | 37.686 | 66.813 | 38.081 | 1.00 | 84.56 | AAAA | C |
| ATOM | 3864 | CE3 | TRP | 404 | 37.703 | 66.710 | 40.506 | 1.00 | 80.95 | AAAA | C |
| ATOM | 3865 | CD1 | TRP | 404 | 36.460 | 68.622 | 37.694 | 1.00 | 83.37 | AAAA | C |
| ATOM | 3866 | HE1 | TRP | 404 | 37.165 | 67.617 | 37.111 | 1.00 | 80.33 | AAAA | H |
| ATOM | 3868 | CS2 | TRP | 404 | 38.477 | 65.662 | 37.982 | 1.00 | 85.91 | AAAA | C |
| ATOM | 3869 | CD3 | TRP | 404 | 38.471 | 65.573 | 40.392 | 1.00 | 86.36 | AAAA | C |
| ATOM | 3870 | CH2 | TRP | 404 | 38.860 | 65.051 | 39.133 | 1.00 | 85.05 | AAAA | C |
| ATOM | 3871 | C | TRP | 404 | 35.034 | 69.517 | 42.420 | 1.00 | 81.60 | AAAA | C |
| ATOM | 3872 | O | TRP | 404 | 35.387 | 70.709 | 42.504 | 1.00 | 84.57 | AAAA | O |
| ATOM | 3873 | H | ASP | 405 | 34.281 | 69.063 | 43.393 | 1.00 | 84.45 | AAAA | H |
| ATOM | 3875 | CA | ASP | 405 | 33.771 | 69.861 | 44.496 | 1.00 | 87.48 | AAAA | C |
| ATOM | 3876 | CB | ASP | 405 | 32.352 | 70.365 | 44.262 | 1.00 | 88.04 | AAAA | C |
| ATOM | 3877 | CG | ASP | 405 | 32.274 | 71.612 | 43.409 | 1.00 | 92.54 | AAAA | C |
| ATOM | 3878 | CD1 | ASP | 405 | 33.306 | 72.285 | 43.207 | 1.00 | 94.82 | AAAA | O |
| ATOM | 3879 | OD2 | ASP | 405 | 31.130 | 71.954 | 42.955 | 1.00 | 95.26 | AAAA | O |
| ATOM | 3880 | C | ASP | 405 | 33.730 | 68.906 | 45.693 | 1.00 | 87.80 | AAAA | C |
| ATOM | 3881 | O | ASP | 405 | 34.245 | 69.224 | 46.743 | 1.00 | 92.19 | AAAA | O |
| ATOM | 3882 | H | ALA | 406 | 33.239 | 67.709 | 45.460 | 1.00 | 84.45 | AAAA | H |
| ATOM | 3884 | CA | ALA | 406 | 33.176 | 66.671 | 46.451 | 1.00 | 82.57 | AAAA | C |
| ATOM | 3885 | CB | ALA | 406 | 31.943 | 68.905 | 46.133 | 1.00 | 76.32 | AAAA | C |
| ATOM | 3886 | C | ALA | 406 | 34.445 | 68.340 | 46.459 | 1.00 | 85.77 | AAAA | C |
| ATOM | 3887 | O | ALA | 406 | 34.470 | 64.923 | 47.185 | 1.00 | 89.38 | AAAA | O |
| ATOM | 3889 | H | ARG | 407 | 35.433 | 66.073 | 45.577 | 1.00 | 83.74 | AAAA | H |
| ATOM | 3890 | CA | ARG | 407 | 36.541 | 65.151 | 45.400 | 1.00 | 79.60 | AAAA | C |
| ATOM | 3891 | CB | ARG | 407 | 36.165 | 64.140 | 44.297 | 1.00 | 77.84 | AAAA | C |
| ATOM | 3892 | CG | ARG | 407 | 35.457 | 62.950 | 44.921 | 1.00 | 81.91 | AAAA | C |
| ATOM | 3893 | CD | ARG | 407 | 35.362 | 61.688 | 44.113 | 1.00 | 86.97 | AAAA | C |
| ATOM | 3894 | HE | ARG | 407 | 36.281 | 60.660 | 44.607 | 1.00 | 86.94 | AAAA | N |
| ATOM | 3896 | CS | ARG | 407 | 37.564 | 60.583 | 44.279 | 1.00 | 92.14 | AAAA | C |
| ATOM | 3897 | NH1 | ARG | 407 | 38.169 | 61.441 | 43.469 | 1.00 | 97.06 | AAAA | H |
| ATOM | 3900 | NH2 | ARG | 407 | 38.309 | 59.616 | 44.770 | 1.00 | 96.33 | AAAA | H |
| ATOM | 3903 | C | ARG | 407 | 37.880 | 65.749 | 45.048 | 1.00 | 76.72 | AAAA | C |
| ATOM | 3904 | O | ARG | 407 | 37.989 | 66.774 | 44.410 | 1.00 | 77.47 | AAAA | O |
| ATOM | 3905 | H | ASN | 408 | 38.958 | 65.081 | 45.453 | 1.00 | 75.75 | AAAA | H |
| ATOM | 3907 | CA | ASN | 408 | 40.311 | 65.556 | 45.173 | 1.00 | 73.79 | AAAA | C |
| ATOM | 3908 | CB | ASN | 408 | 40.938 | 66.240 | 46.388 | 1.00 | 74.45 | AAAA | C |
| ATOM | 3909 | CG | ASN | 408 | 41.986 | 67.242 | 45.947 | 1.00 | 82.51 | AAAA | C |
| ATOM | 3910 | OD1 | ASN | 408 | 41.813 | 68.429 | 46.240 | 1.00 | 90.33 | AAAA | O |
| ATOM | 3911 | ND2 | ASN | 408 | 43.028 | 66.821 | 45.253 | 1.00 | 84.45 | AAAA | N |
| ATOM | 3914 | C | ASN | 408 | 41.257 | 64.468 | 44.654 | 1.00 | 65.97 | AAAA | C |
| ATOM | 3915 | O | ASN | 408 | 41.251 | 63.374 | 45.151 | 1.00 | 63.82 | AAAA | O |
| ATOM | 3916 | N | LEU | 409 | 42.041 | 64.793 | 43.650 | 1.00 | 61.41 | AAAA | H |
| ATOM | 3918 | CA | LEU | 409 | 42.896 | 63.872 | 42.947 | 1.00 | 60.90 | AAAA | C |
| ATOM | 3919 | CB | LEU | 409 | 42.153 | 63.250 | 41.768 | 1.00 | 62.98 | AAAA | C |
| ATOM | 3920 | CG | LEU | 409 | 42.992 | 62.553 | 40.704 | 1.00 | 59.77 | AAAA | C |
| ATOM | 3921 | CD1 | LEU | 409 | 43.488 | 61.205 | 41.197 | 1.00 | 54.06 | AAAA | C |
| ATOM | 3922 | CD2 | LEU | 409 | 42.094 | 62.445 | 39.486 | 1.00 | 55.74 | AAAA | C |
| ATOM | 3923 | C | LEU | 409 | 44.151 | 64.599 | 42.485 | 1.00 | 61.19 | AAAA | C |
| ATOM | 3924 | O | LEU | 409 | 44.141 | 65.809 | 42.370 | 1.00 | 60.64 | AAAA | O |
| ATOM | 3925 | H | THR | 410 | 45.281 | 63.903 | 42.424 | 1.00 | 63.74 | AAAA | H |
| ATOM | 3927 | CA | THR | 410 | 46.588 | 64.462 | 42.131 | 1.00 | 60.44 | AAAA | C |
| ATOM | 3928 | CB | THR | 410 | 47.454 | 64.676 | 43.385 | 1.00 | 67.08 | AAAA | C |
| ATOM | 3929 | OG1 | THR | 410 | 46.870 | 65.746 | 44.157 | 1.00 | 74.29 | AAAA | O |
| ATOM | 3931 | CG2 | THR | 410 | 48.909 | 65.103 | 43.162 | 1.00 | 48.56 | AAAA | C |
| ATOM | 3932 | C | THR | 410 | 47.426 | 63.565 | 41.218 | 1.00 | 56.62 | AAAA | C |
| ATOM | 3933 | O | THR | 410 | 47.382 | 62.354 | 41.317 | 1.00 | 54.99 | AAAA | O |
| ATOM | 3934 | H | ILE | 411 | 48.077 | 64.245 | 40.288 | 1.00 | 53.97 | AAAA | H |
| ATOM | 3936 | CA | ILE | 411 | 48.897 | 63.562 | 39.291 | 1.00 | 53.29 | AAAA | C |

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|------|------|----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOH | 3937 | CB | ILE | 411 | 49.409 | 63.854 | 37.864 | 1.00 | 49.81 | AAAA | C |
| ATOH | 3938 | CG | ILE | 411 | 49.216 | 63.128 | 36.806 | 1.00 | 30.86 | AAAA | C |
| ATOH | 3939 | CG | ILE | 411 | 46.911 | 63.489 | 37.729 | 1.00 | 40.83 | AAAA | C |
| ATOH | 3940 | CD | ILE | 411 | 46.322 | 63.547 | 36.338 | 1.00 | 38.51 | AAAA | C |
| ATOH | 3941 | C | ILE | 411 | 50.319 | 64.018 | 39.568 | 1.00 | 55.38 | AAAA | C |
| ATOH | 3942 | O | ILE | 411 | 50.656 | 65.179 | 39.291 | 1.00 | 57.59 | AAAA | O |
| ATOH | 3943 | H | SER | 412 | 51.073 | 63.182 | 40.270 | 1.00 | 54.26 | AAAA | H |
| ATOH | 3945 | CA | SER | 412 | 52.434 | 63.502 | 40.689 | 1.00 | 54.46 | AAAA | C |
| ATOH | 3946 | CB | SER | 412 | 53.071 | 62.210 | 41.248 | 1.00 | 55.78 | AAAA | C |
| ATOH | 3947 | CG | SER | 412 | 53.756 | 62.536 | 42.434 | 1.00 | 67.12 | AAAA | O |
| ATOH | 3949 | C | SER | 412 | 53.326 | 63.910 | 39.523 | 1.00 | 55.52 | AAAA | C |
| ATOH | 3950 | O | SER | 412 | 54.081 | 64.876 | 39.527 | 1.00 | 55.04 | AAAA | O |
| ATOH | 3951 | H | ALA | 413 | 53.254 | 63.124 | 38.438 | 1.00 | 50.12 | AAAA | H |
| ATOH | 3953 | CA | ALA | 413 | 54.064 | 63.402 | 37.281 | 1.00 | 50.01 | AAAA | C |
| ATOH | 3954 | CB | ALA | 413 | 55.334 | 62.520 | 37.365 | 1.00 | 34.96 | AAAA | C |
| ATOH | 3955 | C | ALA | 413 | 53.301 | 63.078 | 35.994 | 1.00 | 48.71 | AAAA | C |
| ATOH | 3956 | O | ALA | 413 | 52.495 | 62.168 | 35.998 | 1.00 | 48.81 | AAAA | O |
| ATOH | 3957 | H | GLY | 414 | 53.675 | 63.690 | 34.895 | 1.00 | 47.92 | AAAA | H |
| ATOH | 3959 | CA | GLY | 414 | 53.057 | 63.454 | 33.607 | 1.00 | 51.75 | AAAA | C |
| ATOH | 3960 | C | GLY | 414 | 52.017 | 64.524 | 33.294 | 1.00 | 52.77 | AAAA | C |
| ATOH | 3961 | O | GLY | 414 | 51.684 | 65.370 | 34.114 | 1.00 | 53.23 | AAAA | O |
| ATOH | 3962 | H | LYS | 415 | 51.385 | 64.406 | 32.138 | 1.00 | 56.31 | AAAA | H |
| ATOH | 3964 | CA | LYS | 415 | 50.289 | 65.317 | 31.759 | 1.00 | 52.49 | AAAA | C |
| ATOH | 3965 | CB | LYS | 415 | 50.884 | 66.358 | 30.833 | 1.00 | 50.94 | AAAA | C |
| ATOH | 3966 | CG | LYS | 415 | 51.198 | 65.855 | 29.429 | 1.00 | 54.39 | AAAA | C |
| ATOH | 3967 | CD | LYS | 415 | 52.288 | 66.691 | 28.765 | 1.00 | 53.96 | AAAA | C |
| ATOH | 3968 | CE | LYS | 415 | 52.785 | 66.151 | 27.441 | 1.00 | 56.01 | AAAA | C |
| ATOH | 3969 | HC | LYS | 415 | 52.426 | 67.032 | 26.284 | 1.00 | 66.36 | AAAA | H |
| ATOH | 3973 | C | LYS | 415 | 49.110 | 64.576 | 31.155 | 1.00 | 50.04 | AAAA | C |
| ATOH | 3974 | O | LYS | 415 | 49.077 | 63.337 | 31.036 | 1.00 | 49.77 | AAAA | O |
| ATOH | 3975 | H | MET | 416 | 48.091 | 65.353 | 30.771 | 1.00 | 48.34 | AAAA | H |
| ATOH | 3977 | CA | MET | 416 | 46.890 | 64.734 | 30.186 | 1.00 | 46.77 | AAAA | C |
| ATOH | 3978 | CB | MET | 416 | 45.629 | 65.186 | 30.949 | 1.00 | 42.79 | AAAA | C |
| ATOH | 3979 | CG | MET | 416 | 45.836 | 65.880 | 32.273 | 1.00 | 40.91 | AAAA | C |
| ATOH | 3980 | SD | MET | 416 | 44.511 | 65.636 | 33.517 | 1.00 | 56.20 | AAAA | S |
| ATOH | 3981 | CE | MET | 416 | 44.002 | 67.365 | 33.690 | 1.00 | 35.94 | AAAA | C |
| ATOH | 3982 | C | MET | 416 | 46.623 | 65.064 | 28.723 | 1.00 | 40.40 | AAAA | C |
| ATOH | 3983 | O | MET | 416 | 46.963 | 66.137 | 28.247 | 1.00 | 34.94 | AAAA | O |
| ATOH | 3984 | H | TYR | 417 | 45.893 | 64.169 | 29.104 | 1.00 | 38.49 | AAAA | H |
| ATOH | 3986 | CA | TYR | 417 | 45.355 | 64.387 | 26.765 | 1.00 | 39.50 | AAAA | C |
| ATOH | 3987 | CB | TYR | 417 | 46.156 | 63.471 | 25.831 | 1.00 | 32.02 | AAAA | C |
| ATOH | 3988 | CG | TYR | 417 | 45.583 | 63.430 | 24.428 | 1.00 | 39.48 | AAAA | C |
| ATOH | 3989 | CD | TYR | 417 | 45.730 | 64.501 | 23.511 | 1.00 | 39.29 | AAAA | C |
| ATOH | 3990 | CE | TYR | 417 | 45.196 | 64.409 | 22.253 | 1.00 | 34.56 | AAAA | C |
| ATOH | 3991 | CD | TYR | 417 | 44.894 | 62.321 | 24.065 | 1.00 | 36.91 | AAAA | C |
| ATOH | 3992 | CE | TYR | 417 | 44.379 | 62.241 | 22.722 | 1.00 | 39.90 | AAAA | C |
| ATOH | 3993 | CG | TYR | 417 | 44.535 | 63.292 | 21.872 | 1.00 | 44.20 | AAAA | C |
| ATOH | 3994 | CH | TYR | 417 | 44.053 | 63.361 | 20.552 | 1.00 | 58.10 | AAAA | O |
| ATOH | 3996 | C | TYR | 417 | 43.853 | 64.065 | 26.699 | 1.00 | 44.18 | AAAA | C |
| ATOH | 3997 | O | TYR | 417 | 43.376 | 62.974 | 27.135 | 1.00 | 42.19 | AAAA | O |
| ATOH | 3998 | H | PHE | 419 | 43.068 | 64.971 | 26.100 | 1.00 | 45.94 | AAAA | H |
| ATOH | 4000 | CA | PHE | 419 | 41.644 | 64.701 | 25.919 | 1.00 | 45.87 | AAAA | C |
| ATOH | 4001 | CB | PHE | 419 | 40.772 | 65.657 | 26.730 | 1.00 | 47.19 | AAAA | C |
| ATOH | 4002 | CG | PHE | 418 | 40.675 | 65.264 | 28.177 | 1.00 | 43.44 | AAAA | C |
| ATOH | 4003 | CD | PHE | 418 | 41.552 | 65.685 | 29.132 | 1.00 | 38.43 | AAAA | C |
| ATOH | 4004 | CD | PHE | 418 | 39.638 | 64.417 | 28.544 | 1.00 | 51.21 | AAAA | C |
| ATOH | 4005 | CE | PHE | 418 | 41.402 | 65.291 | 30.440 | 1.00 | 46.44 | AAAA | C |
| ATOH | 4006 | CE | PHE | 418 | 39.486 | 64.023 | 29.845 | 1.00 | 46.63 | AAAA | C |
| ATOH | 4007 | CD | PHE | 418 | 40.358 | 64.454 | 30.801 | 1.00 | 44.68 | AAAA | C |
| ATOH | 4008 | C | PHE | 418 | 41.251 | 64.730 | 24.440 | 1.00 | 44.64 | AAAA | C |
| ATOH | 4009 | O | PHE | 418 | 41.375 | 65.762 | 23.812 | 1.00 | 47.60 | AAAA | O |
| ATOH | 4010 | N | ALA | 419 | 40.554 | 63.713 | 23.936 | 1.00 | 43.06 | AAAA | N |
| ATOH | 4012 | CA | ALA | 419 | 40.015 | 63.793 | 22.607 | 1.00 | 39.21 | AAAA | C |
| ATOH | 4013 | CB | ALA | 419 | 41.090 | 63.562 | 21.555 | 1.00 | 30.88 | AAAA | C |
| ATOH | 4014 | C | ALA | 419 | 38.837 | 62.846 | 22.366 | 1.00 | 41.77 | AAAA | C |
| ATOH | 4015 | O | ALA | 419 | 38.871 | 61.629 | 22.557 | 1.00 | 36.08 | AAAA | O |
| ATOH | 4016 | N | PHE | 420 | 37.829 | 63.398 | 21.618 | 1.00 | 40.41 | AAAA | N |
| ATOH | 4018 | CA | PHE | 420 | 36.742 | 62.621 | 21.070 | 1.00 | 40.03 | AAAA | C |
| ATOH | 4019 | CB | PHE | 420 | 37.157 | 61.430 | 20.180 | 1.00 | 45.54 | AAAA | C |
| ATOH | 4020 | CG | PHE | 420 | 37.832 | 61.909 | 18.912 | 1.00 | 54.18 | AAAA | C |
| ATOH | 4021 | CD | PHE | 420 | 39.221 | 61.987 | 18.751 | 1.00 | 49.23 | AAAA | C |
| ATOH | 4022 | CD | PHE | 420 | 37.006 | 62.345 | 17.871 | 1.00 | 47.65 | AAAA | C |
| ATOH | 4023 | CE | PHE | 420 | 39.783 | 62.496 | 17.567 | 1.00 | 46.00 | AAAA | C |
| ATOH | 4024 | CE | PHE | 420 | 37.572 | 62.833 | 16.725 | 1.00 | 51.10 | AAAA | C |
| ATOH | 4025 | CS | PHE | 420 | 38.964 | 62.928 | 16.549 | 1.00 | 44.01 | AAAA | C |
| ATOH | 4026 | C | PHE | 420 | 35.762 | 62.146 | 22.126 | 1.00 | 41.65 | AAAA | C |
| ATOH | 4027 | O | PHE | 420 | 35.352 | 60.991 | 22.215 | 1.00 | 38.35 | AAAA | O |
| ATOH | 4028 | N | ASN | 421 | 35.459 | 63.024 | 23.049 | 1.00 | 45.35 | AAAA | N |
| ATOH | 4030 | CA | ASN | 421 | 34.477 | 62.960 | 24.112 | 1.00 | 46.86 | AAAA | C |
| ATOH | 4031 | CB | ASN | 421 | 35.183 | 63.276 | 25.449 | 1.00 | 43.60 | AAAA | C |
| ATOH | 4032 | CG | ASN | 421 | 36.407 | 62.401 | 25.654 | 1.00 | 47.90 | AAAA | C |
| ATOH | 4033 | OD | ASN | 421 | 36.426 | 61.147 | 25.714 | 1.00 | 44.83 | AAAA | O |
| ATOH | 4034 | ND | ASN | 421 | 37.541 | 63.101 | 25.732 | 1.00 | 37.46 | AAAA | N |
| ATOH | 4037 | C | ASN | 421 | 33.432 | 64.069 | 23.835 | 1.00 | 47.83 | AAAA | C |
| ATOH | 4038 | O | ASN | 421 | 33.617 | 65.233 | 24.237 | 1.00 | 38.85 | AAAA | O |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 4039 | H | PRO | 422 | 32.453 | 63.777 | 22.968 | 1.00 | 47.86 | AAAA | H |
| ATOM | 4040 | CD | PRO | 422 | 32.213 | 62.423 | 22.372 | 1.00 | 44.11 | AAAA | C |
| ATOM | 4041 | CA | PRO | 422 | 31.463 | 64.776 | 22.605 | 1.00 | 47.85 | AAAA | C |
| ATOM | 4042 | CB | PRO | 422 | 30.731 | 64.084 | 21.446 | 1.00 | 44.86 | AAAA | C |
| ATOM | 4043 | CG | PRO | 422 | 30.947 | 62.623 | 21.606 | 1.00 | 43.01 | AAAA | C |
| ATOM | 4044 | C | PRO | 422 | 30.577 | 65.284 | 23.735 | 1.00 | 51.16 | AAAA | C |
| ATOM | 4045 | O | PRO | 422 | 30.223 | 66.486 | 23.744 | 1.00 | 48.54 | AAAA | O |
| ATOM | 4046 | H | LYS | 423 | 30.320 | 64.487 | 24.774 | 1.00 | 52.90 | AAAA | N |
| ATOM | 4048 | CA | LYS | 423 | 29.431 | 64.908 | 25.865 | 1.00 | 58.82 | AAAA | C |
| ATOM | 4049 | CB | LYS | 423 | 28.556 | 63.721 | 26.360 | 1.00 | 52.93 | AAAA | C |
| ATOM | 4050 | CG | LYS | 423 | 28.209 | 62.810 | 25.196 | 1.00 | 70.55 | AAAA | C |
| ATOM | 4051 | CD | LYS | 423 | 26.743 | 62.448 | 24.996 | 1.00 | 73.79 | AAAA | C |
| ATOM | 4052 | CE | LYS | 423 | 26.030 | 63.374 | 24.021 | 1.00 | 77.06 | AAAA | C |
| ATOM | 4053 | NE | LYS | 423 | 25.949 | 64.748 | 24.614 | 1.00 | 64.99 | AAAA | N |
| ATOM | 4057 | C | LYS | 423 | 30.158 | 65.482 | 27.071 | 1.00 | 57.43 | AAAA | C |
| ATOM | 4058 | O | LYS | 423 | 29.582 | 65.478 | 28.152 | 1.00 | 55.22 | AAAA | O |
| ATOM | 4059 | H | LEU | 424 | 31.425 | 65.859 | 26.862 | 1.00 | 55.95 | AAAA | H |
| ATOM | 4061 | CA | LEU | 424 | 32.261 | 66.162 | 28.017 | 1.00 | 57.07 | AAAA | C |
| ATOM | 4062 | CB | LEU | 424 | 33.463 | 65.250 | 28.237 | 1.00 | 49.16 | AAAA | C |
| ATOM | 4063 | CG | LEU | 424 | 34.390 | 65.748 | 29.370 | 1.00 | 68.27 | AAAA | C |
| ATOM | 4064 | CD1 | LEU | 424 | 33.821 | 65.362 | 30.734 | 1.00 | 60.66 | AAAA | C |
| ATOM | 4065 | CD2 | LEU | 424 | 35.825 | 65.276 | 29.123 | 1.00 | 60.35 | AAAA | C |
| ATOM | 4066 | C | LEU | 424 | 32.709 | 67.585 | 27.878 | 1.00 | 56.29 | AAAA | C |
| ATOM | 4067 | O | LEU | 424 | 33.696 | 67.861 | 27.201 | 1.00 | 59.98 | AAAA | O |
| ATOM | 4068 | H | CYS | 425 | 31.995 | 68.488 | 28.492 | 1.00 | 58.76 | AAAA | H |
| ATOM | 4070 | CA | CYS | 425 | 32.342 | 69.916 | 28.406 | 1.00 | 60.39 | AAAA | C |
| ATOM | 4071 | C | CYS | 425 | 33.771 | 70.119 | 28.810 | 1.00 | 62.59 | AAAA | C |
| ATOM | 4072 | O | CYS | 425 | 34.288 | 69.665 | 29.831 | 1.00 | 64.45 | AAAA | O |
| ATOM | 4073 | CB | CYS | 425 | 31.249 | 70.644 | 29.214 | 1.00 | 68.23 | AAAA | C |
| ATOM | 4074 | SG | CYS | 425 | 29.916 | 71.303 | 28.086 | 1.00 | 81.03 | AAAA | S |
| ATOM | 4075 | H | VAL | 426 | 34.529 | 70.953 | 28.102 | 1.00 | 65.31 | AAAA | H |
| ATOM | 4077 | CA | VAL | 426 | 35.943 | 71.149 | 28.358 | 1.00 | 65.49 | AAAA | C |
| ATOM | 4078 | CB | VAL | 426 | 36.644 | 72.022 | 27.310 | 1.00 | 66.66 | AAAA | C |
| ATOM | 4079 | CG1 | VAL | 426 | 36.715 | 71.413 | 25.925 | 1.00 | 62.49 | AAAA | C |
| ATOM | 4080 | CG2 | VAL | 426 | 35.962 | 73.365 | 27.239 | 1.00 | 60.92 | AAAA | C |
| ATOM | 4081 | C | VAL | 426 | 36.105 | 71.711 | 29.757 | 1.00 | 65.99 | AAAA | C |
| ATOM | 4082 | O | VAL | 426 | 37.180 | 71.724 | 30.388 | 1.00 | 64.51 | AAAA | O |
| ATOM | 4083 | H | SER | 427 | 35.090 | 72.361 | 30.267 | 1.00 | 67.67 | AAAA | H |
| ATOM | 4085 | CA | SER | 427 | 35.091 | 72.927 | 31.599 | 1.00 | 66.85 | AAAA | C |
| ATOM | 4086 | CB | SER | 427 | 33.685 | 73.499 | 31.864 | 1.00 | 61.16 | AAAA | C |
| ATOM | 4087 | CG | SER | 427 | 34.088 | 74.660 | 32.098 | 1.00 | 67.05 | AAAA | O |
| ATOM | 4089 | C | SER | 427 | 35.515 | 71.972 | 32.701 | 1.00 | 64.24 | AAAA | C |
| ATOM | 4090 | O | SER | 427 | 36.332 | 72.328 | 33.573 | 1.00 | 63.66 | AAAA | O |
| ATOM | 4091 | H | GLU | 428 | 34.965 | 70.771 | 32.618 | 1.00 | 58.75 | AAAA | H |
| ATOM | 4093 | CA | GLU | 428 | 35.384 | 69.753 | 33.585 | 1.00 | 63.39 | AAAA | C |
| ATOM | 4094 | CB | GLU | 428 | 34.594 | 68.495 | 33.240 | 1.00 | 68.67 | AAAA | C |
| ATOM | 4095 | CG | GLU | 428 | 33.115 | 68.560 | 33.537 | 1.00 | 66.59 | AAAA | C |
| ATOM | 4096 | CD | GLU | 428 | 32.785 | 68.560 | 35.023 | 1.00 | 72.33 | AAAA | C |
| ATOM | 4097 | CE1 | GLU | 428 | 32.729 | 67.522 | 35.722 | 1.00 | 81.62 | AAAA | C |
| ATOM | 4098 | CE2 | GLU | 428 | 32.581 | 69.698 | 35.517 | 1.00 | 70.97 | AAAA | O |
| ATOM | 4099 | C | GLU | 428 | 36.970 | 69.485 | 33.429 | 1.00 | 61.63 | AAAA | C |
| ATOM | 4100 | O | GLU | 428 | 37.671 | 69.696 | 34.307 | 1.00 | 62.03 | AAAA | O |
| ATOM | 4101 | H | ILE | 429 | 37.265 | 69.262 | 32.165 | 1.00 | 61.26 | AAAA | H |
| ATOM | 4103 | CA | ILE | 429 | 38.631 | 69.038 | 31.789 | 1.00 | 61.09 | AAAA | C |
| ATOM | 4104 | CB | ILE | 429 | 38.759 | 68.933 | 30.263 | 1.00 | 59.32 | AAAA | C |
| ATOM | 4105 | CG2 | ILE | 429 | 40.257 | 68.915 | 29.895 | 1.00 | 45.93 | AAAA | C |
| ATOM | 4106 | CG1 | ILE | 429 | 37.968 | 67.719 | 29.794 | 1.00 | 57.66 | AAAA | C |
| ATOM | 4107 | CD1 | ILE | 429 | 38.038 | 67.555 | 28.285 | 1.00 | 53.49 | AAAA | C |
| ATOM | 4108 | C | ILE | 429 | 39.498 | 70.166 | 32.323 | 1.00 | 61.90 | AAAA | C |
| ATOM | 4109 | O | ILE | 429 | 40.592 | 70.017 | 32.867 | 1.00 | 61.28 | AAAA | O |
| ATOM | 4110 | H | TYR | 430 | 38.987 | 71.384 | 32.200 | 1.00 | 65.34 | AAAA | H |
| ATOM | 4112 | CA | TYR | 430 | 39.729 | 72.543 | 32.719 | 1.00 | 68.10 | AAAA | C |
| ATOM | 4113 | CB | TYR | 430 | 39.180 | 73.822 | 32.099 | 1.00 | 71.02 | AAAA | C |
| ATOM | 4114 | CG | TYR | 430 | 39.538 | 74.006 | 30.639 | 1.00 | 75.98 | AAAA | C |
| ATOM | 4115 | CD1 | TYR | 430 | 38.653 | 73.821 | 29.599 | 1.00 | 77.60 | AAAA | C |
| ATOM | 4116 | CE1 | TYR | 430 | 38.953 | 73.977 | 28.270 | 1.00 | 75.72 | AAAA | C |
| ATOM | 4117 | CD2 | TYR | 430 | 40.810 | 74.401 | 30.260 | 1.00 | 75.95 | AAAA | C |
| ATOM | 4118 | CE2 | TYR | 430 | 41.155 | 74.575 | 28.937 | 1.00 | 74.81 | AAAA | C |
| ATOM | 4119 | CE | TYR | 430 | 40.221 | 74.359 | 27.952 | 1.00 | 78.51 | AAAA | C |
| ATOM | 4120 | OH | TYR | 430 | 40.564 | 74.542 | 26.616 | 1.00 | 85.40 | AAAA | O |
| ATOM | 4122 | C | TYR | 430 | 39.779 | 72.634 | 34.241 | 1.00 | 63.72 | AAAA | C |
| ATOM | 4123 | O | TYR | 430 | 40.654 | 73.321 | 34.758 | 1.00 | 58.26 | AAAA | O |
| ATOM | 4124 | H | ARG | 431 | 38.819 | 72.017 | 34.907 | 1.00 | 65.53 | AAAA | H |
| ATOM | 4126 | CA | ARG | 431 | 38.747 | 72.043 | 36.356 | 1.00 | 68.15 | AAAA | C |
| ATOM | 4127 | CB | ARG | 431 | 37.348 | 71.748 | 36.898 | 1.00 | 73.32 | AAAA | C |
| ATOM | 4128 | CG | ARG | 431 | 37.345 | 71.815 | 38.430 | 1.00 | 82.99 | AAAA | C |
| ATOM | 4129 | CD | ARG | 431 | 37.270 | 73.279 | 38.860 | 1.00 | 88.39 | AAAA | C |
| ATOM | 4130 | HE | ARG | 431 | 37.698 | 73.472 | 40.258 | 1.00 | 92.48 | AAAA | N |
| ATOM | 4132 | CZ | ARG | 431 | 36.835 | 73.258 | 41.259 | 1.00 | 94.93 | AAAA | C |
| ATOM | 4133 | HH1 | ARG | 431 | 35.610 | 72.872 | 40.872 | 1.00 | 87.40 | AAAA | N |
| ATOM | 4136 | HH2 | ARG | 431 | 37.021 | 73.371 | 42.567 | 1.00 | 95.17 | AAAA | N |
| ATOM | 4139 | C | ARG | 431 | 39.718 | 70.986 | 36.877 | 1.00 | 67.75 | AAAA | C |
| ATOM | 4140 | O | ARG | 431 | 40.637 | 71.292 | 37.629 | 1.00 | 66.74 | AAAA | O |
| ATOM | 4141 | H | MET | 432 | 39.541 | 69.791 | 36.305 | 1.00 | 63.87 | AAAA | H |
| ATOM | 4143 | CA | MET | 432 | 40.437 | 68.703 | 36.652 | 1.00 | 64.40 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 4144 | UR | HET | 432 | 40.237 | 67.522 | 35.718 | 1.00 | 54.25 | AAAA | C |
| ATOM | 4145 | CG | HET | 432 | 41.254 | 66.426 | 35.971 | 1.00 | 40.18 | AAAA | C |
| ATOM | 4146 | SD | HET | 432 | 40.829 | 64.925 | 35.112 | 1.00 | 52.21 | AAAA | S |
| ATOM | 4147 | CE | HET | 432 | 41.582 | 63.681 | 36.137 | 1.00 | 54.89 | AAAA | C |
| ATOM | 4148 | C | HET | 432 | 41.891 | 69.170 | 36.626 | 1.00 | 64.65 | AAAA | C |
| ATOM | 4149 | O | HET | 432 | 42.530 | 68.992 | 37.653 | 1.00 | 65.88 | AAAA | O |
| ATOM | 4150 | H | GLU | 433 | 42.331 | 69.811 | 35.556 | 1.00 | 65.78 | AAAA | N |
| ATOM | 4152 | CA | GLU | 433 | 43.622 | 70.469 | 35.510 | 1.00 | 69.16 | AAAA | C |
| ATOM | 4153 | CB | GLU | 433 | 43.704 | 71.506 | 34.401 | 1.00 | 69.58 | AAAA | C |
| ATOM | 4154 | CG | GLU | 433 | 44.121 | 70.967 | 33.048 | 1.00 | 76.91 | AAAA | C |
| ATOM | 4155 | CD | GLU | 433 | 44.623 | 72.149 | 32.242 | 1.00 | 82.02 | AAAA | C |
| ATOM | 4156 | OE1 | GLU | 433 | 44.718 | 73.224 | 32.874 | 1.00 | 86.82 | AAAA | O |
| ATOM | 4157 | OE2 | GLU | 433 | 44.905 | 72.050 | 31.042 | 1.00 | 88.26 | AAAA | O |
| ATOM | 4158 | C | GLU | 433 | 44.016 | 71.219 | 36.781 | 1.00 | 71.29 | AAAA | C |
| ATOM | 4159 | O | GLU | 433 | 45.133 | 71.083 | 37.294 | 1.00 | 74.29 | AAAA | O |
| ATOM | 4160 | H | GLU | 434 | 43.178 | 72.120 | 37.280 | 1.00 | 72.93 | AAAA | H |
| ATOM | 4162 | CA | GLU | 434 | 43.505 | 72.873 | 38.485 | 1.00 | 72.88 | AAAA | C |
| ATOM | 4163 | CB | GLU | 434 | 42.458 | 73.916 | 38.840 | 1.00 | 81.36 | AAAA | C |
| ATOM | 4164 | CG | GLU | 434 | 41.191 | 73.956 | 38.032 | 1.00 | 83.34 | AAAA | C |
| ATOM | 4165 | CD | GLU | 434 | 40.181 | 75.004 | 38.432 | 1.00 | 97.32 | AAAA | C |
| ATOM | 4166 | OE1 | GLU | 434 | 39.521 | 74.928 | 39.505 | 1.00 | 97.34 | AAAA | O |
| ATOM | 4167 | OE2 | GLU | 434 | 40.080 | 75.941 | 37.583 | 1.00 | 99.95 | AAAA | O |
| ATOM | 4168 | C | GLU | 434 | 43.675 | 71.886 | 39.632 | 1.00 | 71.46 | AAAA | C |
| ATOM | 4169 | O | GLU | 434 | 44.728 | 71.858 | 40.251 | 1.00 | 78.49 | AAAA | O |
| ATOM | 4170 | H | VAL | 435 | 42.670 | 71.095 | 39.926 | 1.00 | 66.34 | AAAA | H |
| ATOM | 4172 | CA | VAL | 435 | 42.711 | 70.129 | 41.001 | 1.00 | 62.49 | AAAA | C |
| ATOM | 4173 | CB | VAL | 435 | 41.451 | 69.217 | 40.972 | 1.00 | 60.38 | AAAA | C |
| ATOM | 4174 | CG1 | VAL | 435 | 41.547 | 68.214 | 42.104 | 1.00 | 52.32 | AAAA | C |
| ATOM | 4175 | CG2 | VAL | 435 | 40.203 | 70.073 | 41.029 | 1.00 | 50.79 | AAAA | C |
| ATOM | 4176 | C | VAL | 435 | 43.939 | 69.253 | 41.018 | 1.00 | 60.74 | AAAA | C |
| ATOM | 4177 | O | VAL | 435 | 44.607 | 69.165 | 42.034 | 1.00 | 62.37 | AAAA | O |
| ATOM | 4178 | H | THR | 436 | 44.282 | 68.506 | 39.988 | 1.00 | 60.67 | AAAA | N |
| ATOM | 4180 | CA | THR | 436 | 45.335 | 67.516 | 39.936 | 1.00 | 56.36 | AAAA | C |
| ATOM | 4181 | CB | THR | 436 | 45.199 | 66.565 | 38.736 | 1.00 | 50.92 | AAAA | C |
| ATOM | 4182 | CG1 | THR | 436 | 44.913 | 67.283 | 37.503 | 1.00 | 47.03 | AAAA | O |
| ATOM | 4184 | CG2 | THR | 436 | 44.108 | 65.526 | 38.901 | 1.00 | 54.38 | AAAA | C |
| ATOM | 4185 | C | THR | 436 | 46.701 | 68.184 | 39.930 | 1.00 | 60.55 | AAAA | C |
| ATOM | 4186 | O | THR | 436 | 47.714 | 67.490 | 40.024 | 1.00 | 60.61 | AAAA | O |
| ATOM | 4187 | H | GLY | 437 | 46.836 | 69.496 | 39.835 | 1.00 | 60.65 | AAAA | H |
| ATOM | 4189 | CA | GLY | 437 | 48.102 | 70.164 | 39.749 | 1.00 | 59.47 | AAAA | C |
| ATOM | 4190 | C | GLY | 437 | 48.800 | 69.964 | 38.424 | 1.00 | 64.78 | AAAA | C |
| ATOM | 4191 | O | GLY | 437 | 49.993 | 70.254 | 38.245 | 1.00 | 62.70 | AAAA | O |
| ATOM | 4192 | H | THR | 438 | 48.112 | 69.387 | 37.390 | 1.00 | 63.79 | AAAA | H |
| ATOM | 4194 | CA | THR | 438 | 48.731 | 69.169 | 36.076 | 1.00 | 65.09 | AAAA | C |
| ATOM | 4195 | CB | THR | 438 | 47.967 | 68.027 | 35.411 | 1.00 | 66.87 | AAAA | C |
| ATOM | 4196 | CG1 | THR | 438 | 46.600 | 69.385 | 35.731 | 1.00 | 62.22 | AAAA | O |
| ATOM | 4199 | CG2 | THR | 438 | 48.209 | 66.659 | 36.619 | 1.00 | 68.74 | AAAA | C |
| ATOM | 4199 | C | THR | 438 | 48.599 | 70.415 | 35.220 | 1.00 | 66.14 | AAAA | C |
| ATOM | 4200 | O | THR | 438 | 49.063 | 70.543 | 34.070 | 1.00 | 69.06 | AAAA | O |
| ATOM | 4201 | H | LYS | 439 | 48.089 | 71.491 | 35.822 | 1.00 | 67.37 | AAAA | H |
| ATOM | 4203 | CA | LYS | 439 | 47.927 | 72.757 | 35.154 | 1.00 | 71.08 | AAAA | C |
| ATOM | 4204 | CB | LYS | 439 | 47.114 | 73.708 | 36.034 | 1.00 | 69.23 | AAAA | C |
| ATOM | 4205 | CG | LYS | 439 | 46.677 | 74.938 | 35.265 | 1.00 | 77.26 | AAAA | C |
| ATOM | 4206 | CD | LYS | 439 | 45.832 | 75.942 | 36.014 | 1.00 | 81.65 | AAAA | C |
| ATOM | 4207 | CE | LYS | 439 | 44.385 | 75.475 | 36.182 | 1.00 | 87.39 | AAAA | C |
| ATOM | 4208 | HZ | LYS | 439 | 43.667 | 76.431 | 37.100 | 1.00 | 93.85 | AAAA | N |
| ATOM | 4212 | C | LYS | 439 | 49.249 | 73.396 | 34.752 | 1.00 | 73.01 | AAAA | C |
| ATOM | 4213 | O | LYS | 439 | 49.996 | 73.986 | 35.541 | 1.00 | 74.60 | AAAA | O |
| ATOM | 4214 | H | GLY | 440 | 49.517 | 73.453 | 33.441 | 1.00 | 73.33 | AAAA | N |
| ATOM | 4216 | CA | GLY | 440 | 50.733 | 74.167 | 33.014 | 1.00 | 71.39 | AAAA | C |
| ATOM | 4217 | C | GLY | 440 | 51.716 | 73.204 | 32.389 | 1.00 | 71.20 | AAAA | C |
| ATOM | 4218 | O | GLY | 440 | 52.684 | 73.650 | 31.822 | 1.00 | 72.70 | AAAA | O |
| ATOM | 4219 | N | ARG | 441 | 51.445 | 71.908 | 32.436 | 1.00 | 72.99 | AAAA | N |
| ATOM | 4221 | CA | ARG | 441 | 52.343 | 70.945 | 31.831 | 1.00 | 74.12 | AAAA | C |
| ATOM | 4222 | CB | ARG | 441 | 52.617 | 69.740 | 32.716 | 1.00 | 69.44 | AAAA | C |
| ATOM | 4223 | CG | ARG | 441 | 51.847 | 69.695 | 34.003 | 1.00 | 63.34 | AAAA | C |
| ATOM | 4224 | CD | ARG | 441 | 52.060 | 68.314 | 34.595 | 1.00 | 67.64 | AAAA | C |
| ATOM | 4225 | HE | ARG | 441 | 52.244 | 68.395 | 36.030 | 1.00 | 61.00 | AAAA | N |
| ATOM | 4227 | CG | ARG | 441 | 52.326 | 67.357 | 36.831 | 1.00 | 59.21 | AAAA | C |
| ATOM | 4228 | NH1 | ARG | 441 | 52.258 | 66.117 | 36.395 | 1.00 | 60.57 | AAAA | N |
| ATOM | 4231 | NH2 | ARG | 441 | 52.468 | 67.596 | 38.128 | 1.00 | 72.94 | AAAA | N |
| ATOM | 4234 | C | ARG | 441 | 51.760 | 70.446 | 30.511 | 1.00 | 73.50 | AAAA | C |
| ATOM | 4235 | O | ARG | 441 | 52.195 | 69.424 | 30.012 | 1.00 | 74.73 | AAAA | O |
| ATOM | 4236 | H | GLN | 442 | 50.732 | 71.114 | 30.043 | 1.00 | 74.69 | AAAA | H |
| ATOM | 4239 | CA | GLN | 442 | 49.959 | 70.646 | 28.914 | 1.00 | 75.13 | AAAA | C |
| ATOM | 4239 | CB | GLN | 442 | 48.457 | 70.875 | 29.126 | 1.00 | 68.73 | AAAA | C |
| ATOM | 4240 | CG | GLN | 442 | 47.669 | 69.576 | 29.195 | 1.00 | 71.20 | AAAA | C |
| ATOM | 4241 | CD | GLN | 442 | 47.623 | 69.028 | 30.607 | 1.00 | 70.98 | AAAA | C |
| ATOM | 4242 | OE1 | GLN | 442 | 47.714 | 67.822 | 30.868 | 1.00 | 78.66 | AAAA | O |
| ATOM | 4243 | NE2 | GLN | 442 | 47.477 | 69.907 | 31.584 | 1.00 | 66.86 | AAAA | N |
| ATOM | 4246 | C | GLN | 442 | 50.326 | 71.359 | 27.627 | 1.00 | 77.69 | AAAA | C |
| ATOM | 4247 | O | GLN | 442 | 50.227 | 72.569 | 27.530 | 1.00 | 75.57 | AAAA | O |
| ATOM | 4248 | H | ALA | 443 | 50.474 | 70.554 | 26.575 | 1.00 | 81.54 | AAAA | N |
| ATOM | 4250 | CA | ALA | 443 | 50.643 | 71.148 | 25.236 | 1.00 | 82.95 | AAAA | C |
| ATOM | 4251 | CB | ALA | 443 | 51.104 | 70.118 | 24.220 | 1.00 | 81.69 | AAAA | C |

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|------|------|-----|-----|-----|--------|--------|--------|------|-------|------|---|
| ATOM | 4252 | C | ALA | 443 | 49.259 | 71.706 | 24.952 | 1.00 | 83.73 | AAAA | C |
| ATOM | 4253 | O | ALA | 443 | 48.398 | 71.744 | 25.930 | 1.00 | 83.87 | AAAA | O |
| ATOM | 4254 | H | LYS | 444 | 48.914 | 72.052 | 23.713 | 1.00 | 86.20 | AAAA | H |
| ATOM | 4256 | CA | LYS | 444 | 47.559 | 72.524 | 23.482 | 1.00 | 85.88 | AAAA | C |
| ATOM | 4257 | CB | LYS | 444 | 47.426 | 73.997 | 23.128 | 1.00 | 83.99 | AAAA | C |
| ATOM | 4258 | CG | LYS | 444 | 46.673 | 74.734 | 24.241 | 1.00 | 93.60 | AAAA | C |
| ATOM | 4259 | CD | LYS | 444 | 45.883 | 73.841 | 25.186 | 1.00 | 95.14 | AAAA | C |
| ATOM | 4260 | CE | LYS | 444 | 46.390 | 73.786 | 26.614 | 1.00 | 97.04 | AAAA | C |
| ATOM | 4261 | NE | LYS | 444 | 45.368 | 73.090 | 27.473 | 1.00 | 97.22 | AAAA | N |
| ATOM | 4265 | C | LYS | 444 | 46.659 | 71.779 | 22.508 | 1.00 | 84.20 | AAAA | C |
| ATOM | 4266 | O | LYS | 444 | 45.428 | 71.901 | 22.635 | 1.00 | 85.63 | AAAA | O |
| ATOM | 4267 | H | GLY | 445 | 47.214 | 70.734 | 21.916 | 1.00 | 78.85 | AAAA | H |
| ATOM | 4269 | CA | GLY | 445 | 46.368 | 69.786 | 21.208 | 1.00 | 75.06 | AAAA | C |
| ATOM | 4270 | C | GLY | 445 | 45.803 | 68.844 | 22.260 | 1.00 | 72.30 | AAAA | C |
| ATOM | 4271 | O | GLY | 445 | 44.963 | 67.993 | 21.940 | 1.00 | 74.90 | AAAA | O |
| ATOM | 4272 | H | ASP | 446 | 46.300 | 68.981 | 23.492 | 1.00 | 67.97 | AAAA | H |
| ATOM | 4274 | CA | ASP | 446 | 45.914 | 68.174 | 24.642 | 1.00 | 62.81 | AAAA | C |
| ATOM | 4275 | CB | ASP | 446 | 46.754 | 68.552 | 25.873 | 1.00 | 55.24 | AAAA | C |
| ATOM | 4276 | CG | ASP | 446 | 48.213 | 68.169 | 25.801 | 1.00 | 54.07 | AAAA | C |
| ATOM | 4277 | OD1 | ASP | 446 | 48.693 | 67.385 | 24.946 | 1.00 | 45.08 | AAAA | O |
| ATOM | 4278 | OD2 | ASP | 446 | 49.091 | 68.595 | 26.593 | 1.00 | 50.12 | AAAA | O |
| ATOM | 4279 | C | ASP | 446 | 44.438 | 68.274 | 25.016 | 1.00 | 58.07 | AAAA | C |
| ATOM | 4280 | O | ASP | 446 | 43.610 | 67.369 | 25.127 | 1.00 | 55.59 | AAAA | O |
| ATOM | 4281 | H | ILE | 447 | 44.043 | 69.527 | 25.226 | 1.00 | 54.13 | AAAA | H |
| ATOM | 4283 | CA | ILE | 447 | 42.652 | 69.822 | 25.510 | 1.00 | 54.09 | AAAA | C |
| ATOM | 4284 | CB | ILE | 447 | 42.505 | 70.502 | 26.877 | 1.00 | 48.92 | AAAA | C |
| ATOM | 4285 | CG2 | ILE | 447 | 41.030 | 70.663 | 27.182 | 1.00 | 41.02 | AAAA | C |
| ATOM | 4286 | CG1 | ILE | 447 | 43.211 | 69.621 | 27.932 | 1.00 | 52.36 | AAAA | C |
| ATOM | 4287 | CD1 | ILE | 447 | 43.468 | 70.329 | 29.237 | 1.00 | 48.47 | AAAA | C |
| ATOM | 4288 | C | ILE | 447 | 42.027 | 70.591 | 24.364 | 1.00 | 53.06 | AAAA | C |
| ATOM | 4289 | O | ILE | 447 | 41.718 | 71.772 | 24.423 | 1.00 | 56.08 | AAAA | O |
| ATOM | 4290 | H | ASN | 448 | 41.625 | 69.915 | 23.307 | 1.00 | 53.17 | AAAA | H |
| ATOM | 4292 | CA | ASN | 448 | 41.013 | 70.642 | 22.202 | 1.00 | 54.61 | AAAA | C |
| ATOM | 4293 | CB | ASN | 448 | 41.283 | 69.982 | 20.863 | 1.00 | 49.17 | AAAA | C |
| ATOM | 4294 | CG | ASN | 448 | 40.415 | 68.786 | 20.577 | 1.00 | 49.40 | AAAA | C |
| ATOM | 4295 | OD1 | ASN | 448 | 39.287 | 68.977 | 20.113 | 1.00 | 52.34 | AAAA | O |
| ATOM | 4296 | ND2 | ASN | 448 | 40.990 | 67.622 | 20.871 | 1.00 | 52.49 | AAAA | N |
| ATOM | 4299 | C | ASN | 448 | 39.518 | 70.824 | 22.402 | 1.00 | 56.44 | AAAA | C |
| ATOM | 4300 | O | ASN | 448 | 38.916 | 69.974 | 22.939 | 1.00 | 55.83 | AAAA | O |
| ATOM | 4301 | H | THR | 449 | 39.071 | 71.917 | 21.764 | 1.00 | 58.52 | AAAA | H |
| ATOM | 4303 | CA | THR | 449 | 37.692 | 72.351 | 21.901 | 1.00 | 58.62 | AAAA | C |
| ATOM | 4304 | CB | THR | 449 | 37.497 | 73.945 | 22.169 | 1.00 | 55.90 | AAAA | C |
| ATOM | 4306 | CG1 | THR | 449 | 37.913 | 74.485 | 20.943 | 1.00 | 68.89 | AAAA | O |
| ATOM | 4307 | CG2 | THR | 449 | 38.354 | 74.352 | 23.310 | 1.00 | 59.06 | AAAA | C |
| ATOM | 4308 | C | THR | 449 | 36.920 | 72.053 | 20.628 | 1.00 | 56.82 | AAAA | C |
| ATOM | 4309 | O | THR | 449 | 35.750 | 72.381 | 20.473 | 1.00 | 60.87 | AAAA | O |
| ATOM | 4310 | H | ARG | 450 | 37.539 | 71.304 | 19.757 | 1.00 | 55.76 | AAAA | H |
| ATOM | 4312 | CA | ARG | 450 | 36.827 | 70.925 | 18.507 | 1.00 | 54.66 | AAAA | C |
| ATOM | 4313 | CB | ARG | 450 | 37.945 | 71.179 | 17.377 | 1.00 | 48.33 | AAAA | C |
| ATOM | 4314 | CG | ARG | 450 | 38.395 | 69.975 | 16.645 | 1.00 | 54.81 | AAAA | C |
| ATOM | 4315 | CD | ARG | 450 | 39.497 | 70.561 | 15.696 | 1.00 | 44.92 | AAAA | C |
| ATOM | 4316 | NE | ARG | 450 | 40.706 | 70.719 | 16.488 | 1.00 | 52.49 | AAAA | N |
| ATOM | 4318 | CG | ARG | 450 | 41.544 | 69.757 | 16.892 | 1.00 | 39.09 | AAAA | C |
| ATOM | 4319 | NH1 | ARG | 450 | 41.176 | 68.572 | 16.466 | 1.00 | 41.07 | AAAA | H |
| ATOM | 4322 | NH2 | ARG | 450 | 42.601 | 70.001 | 17.610 | 1.00 | 45.18 | AAAA | N |
| ATOM | 4325 | C | ARG | 450 | 36.267 | 69.553 | 18.557 | 1.00 | 56.82 | AAAA | C |
| ATOM | 4326 | O | ARG | 450 | 35.186 | 69.303 | 17.992 | 1.00 | 58.15 | AAAA | O |
| ATOM | 4327 | H | ASN | 451 | 36.800 | 68.583 | 19.324 | 1.00 | 56.66 | AAAA | H |
| ATOM | 4329 | CA | ASN | 451 | 36.107 | 67.311 | 19.434 | 1.00 | 50.27 | AAAA | C |
| ATOM | 4330 | CB | ASN | 451 | 36.725 | 66.127 | 18.760 | 1.00 | 48.54 | AAAA | C |
| ATOM | 4331 | CG | ASN | 451 | 38.243 | 66.143 | 18.764 | 1.00 | 60.51 | AAAA | C |
| ATOM | 4332 | OD1 | ASN | 451 | 38.779 | 66.279 | 19.855 | 1.00 | 53.45 | AAAA | O |
| ATOM | 4333 | ND2 | ASN | 451 | 38.707 | 65.976 | 17.506 | 1.00 | 54.88 | AAAA | N |
| ATOM | 4336 | C | ASN | 451 | 35.849 | 66.854 | 20.869 | 1.00 | 52.97 | AAAA | C |
| ATOM | 4337 | O | ASN | 451 | 35.330 | 65.750 | 21.096 | 1.00 | 49.71 | AAAA | O |
| ATOM | 4338 | H | ASN | 452 | 36.126 | 67.668 | 21.851 | 1.00 | 51.98 | AAAA | H |
| ATOM | 4340 | CA | ASN | 452 | 35.769 | 67.485 | 23.229 | 1.00 | 55.88 | AAAA | C |
| ATOM | 4341 | CB | ASN | 452 | 36.947 | 67.873 | 24.136 | 1.00 | 54.62 | AAAA | C |
| ATOM | 4342 | CG | ASN | 452 | 37.936 | 66.736 | 24.285 | 1.00 | 60.96 | AAAA | C |
| ATOM | 4343 | OD1 | ASN | 452 | 37.646 | 65.633 | 24.735 | 1.00 | 51.30 | AAAA | O |
| ATOM | 4344 | ND2 | ASN | 452 | 39.153 | 67.098 | 23.855 | 1.00 | 56.75 | AAAA | N |
| ATOM | 4347 | C | ASN | 452 | 34.603 | 68.385 | 23.688 | 1.00 | 58.11 | AAAA | C |
| ATOM | 4349 | O | ASN | 452 | 34.785 | 69.629 | 23.657 | 1.00 | 55.07 | AAAA | O |
| ATOM | 4349 | H | GLY | 453 | 33.444 | 67.813 | 23.985 | 1.00 | 55.08 | AAAA | H |
| ATOM | 4351 | CA | GLY | 453 | 32.313 | 68.658 | 24.296 | 1.00 | 59.47 | AAAA | C |
| ATOM | 4352 | C | GLY | 453 | 31.500 | 69.269 | 23.174 | 1.00 | 64.95 | AAAA | C |
| ATOM | 4353 | O | GLY | 453 | 30.302 | 69.603 | 23.276 | 1.00 | 65.71 | AAAA | O |
| ATOM | 4354 | N | GLU | 454 | 31.910 | 69.109 | 21.910 | 1.00 | 67.44 | AAAA | N |
| ATOM | 4356 | CA | GLU | 454 | 31.266 | 69.543 | 20.690 | 1.00 | 63.63 | AAAA | C |
| ATOM | 4357 | CB | GLU | 454 | 31.739 | 68.818 | 19.401 | 1.00 | 53.71 | AAAA | C |
| ATOM | 4358 | CG | GLU | 454 | 32.348 | 67.430 | 19.738 | 1.00 | 49.50 | AAAA | C |
| ATOM | 4359 | CD | GLU | 454 | 32.368 | 66.620 | 18.454 | 1.00 | 54.61 | AAAA | C |
| ATOM | 4360 | OE1 | GLU | 454 | 31.368 | 66.637 | 17.702 | 0.01 | 54.10 | AAAA | O |
| ATOM | 4361 | OE2 | GLU | 454 | 33.417 | 66.003 | 18.160 | 0.01 | 54.17 | AAAA | O |
| ATOM | 4362 | C | GLU | 454 | 29.762 | 69.301 | 20.767 | 1.00 | 65.41 | AAAA | C |

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|------|------|------|-----|-----|--------|--------|--------|------|--------|------|---|
| ATOH | 4363 | O | GLU | 454 | 29.022 | 70.089 | 20.163 | 1.00 | 67.86 | AAAA | O |
| ATOH | 4364 | H | ARG | 455 | 29.288 | 68.187 | 21.333 | 1.00 | 66.45 | AAAA | H |
| ATOH | 4366 | CA | ARG | 455 | 27.943 | 67.997 | 21.371 | 1.00 | 69.33 | AAAA | C |
| ATOH | 4367 | CB | ARG | 455 | 27.448 | 66.733 | 20.652 | 1.00 | 73.38 | AAAA | C |
| ATOH | 4368 | CG | ARG | 455 | 28.467 | 65.912 | 19.924 | 1.00 | 74.27 | AAAA | C |
| ATOH | 4369 | CD | ARG | 455 | 27.775 | 64.740 | 19.240 | 1.00 | 79.54 | AAAA | C |
| ATOH | 4370 | HE | ARG | 455 | 27.301 | 63.638 | 20.052 | 1.00 | 86.31 | AAAA | N |
| ATOH | 4372 | CS | ARG | 455 | 27.802 | 62.412 | 20.189 | 1.00 | 88.60 | AAAA | C |
| ATOH | 4373 | IHH1 | ARG | 455 | 28.890 | 61.997 | 19.538 | 1.00 | 84.51 | AAAA | N |
| ATOH | 4376 | IHH2 | ARG | 455 | 27.225 | 61.523 | 21.003 | 1.00 | 87.36 | AAAA | N |
| ATOH | 4379 | C | ARG | 455 | 27.213 | 67.934 | 22.756 | 1.00 | 67.35 | AAAA | C |
| ATOH | 4380 | O | ARG | 455 | 26.423 | 67.025 | 22.961 | 1.00 | 66.26 | AAAA | O |
| ATOH | 4381 | H | ALA | 456 | 27.499 | 68.879 | 23.623 | 1.00 | 66.52 | AAAA | N |
| ATOH | 4383 | CA | ALA | 456 | 26.947 | 68.906 | 24.964 | 1.00 | 72.01 | AAAA | C |
| ATOH | 4384 | CB | ALA | 456 | 27.832 | 68.147 | 25.939 | 1.00 | 61.84 | AAAA | C |
| ATOH | 4385 | C | ALA | 456 | 26.802 | 70.379 | 25.371 | 1.00 | 75.25 | AAAA | C |
| ATOH | 4386 | O | ALA | 456 | 27.706 | 71.219 | 25.202 | 1.00 | 81.30 | AAAA | O |
| ATOH | 4387 | H | SER | 457 | 25.653 | 70.720 | 25.939 | 0.50 | 71.91 | AAAA | H |
| ATOH | 4389 | CA | SER | 457 | 25.431 | 72.095 | 26.358 | 0.50 | 69.64 | AAAA | C |
| ATOH | 4390 | CB | SER | 457 | 23.991 | 72.247 | 26.836 | 0.50 | 73.30 | AAAA | C |
| ATOH | 4391 | OG | SER | 457 | 23.422 | 73.294 | 26.060 | 0.50 | 73.31 | AAAA | O |
| ATOH | 4393 | C | SER | 457 | 26.418 | 72.510 | 27.437 | 0.50 | 69.27 | AAAA | C |
| ATOH | 4394 | O | SER | 457 | 26.458 | 71.957 | 28.530 | 0.50 | 67.32 | AAAA | O |
| ATOH | 4395 | H | CYS | 458 | 27.197 | 73.531 | 27.117 | 0.50 | 70.44 | AAAA | N |
| ATOH | 4397 | CA | CYS | 458 | 28.287 | 73.960 | 27.972 | 0.50 | 72.57 | AAAA | C |
| ATOH | 4398 | C | CYS | 458 | 27.949 | 75.205 | 28.757 | 0.50 | 72.54 | AAAA | C |
| ATOH | 4399 | O | CYS | 458 | 27.065 | 75.128 | 29.606 | 0.50 | 76.63 | AAAA | O |
| ATOH | 4400 | CB | CYS | 458 | 29.527 | 74.171 | 27.089 | 0.50 | 75.38 | AAAA | C |
| ATOH | 4401 | SG | CYS | 458 | 30.844 | 73.032 | 27.490 | 0.50 | 72.18 | AAAA | S |
| ATOH | 4402 | H | ALA | 459 | 28.607 | 76.306 | 28.441 | 0.50 | 70.13 | AAAA | N |
| ATOH | 4404 | CA | ALA | 459 | 28.445 | 77.572 | 29.116 | 0.50 | 70.05 | AAAA | C |
| ATOH | 4405 | CB | ALA | 459 | 27.046 | 78.149 | 28.996 | 0.50 | 70.57 | AAAA | C |
| ATOH | 4406 | C | ALA | 459 | 28.826 | 77.461 | 30.601 | 0.50 | 70.13 | AAAA | C |
| ATOH | 4407 | O | ALA | 459 | 29.080 | 78.556 | 31.154 | 0.50 | 69.96 | AAAA | O |
| ATOH | 4407 | OT | ALA | 459 | 28.856 | 76.301 | 31.054 | 0.50 | 68.22 | AAAA | O |
| ATOH | 4502 | C1 | IAG | 461 | 59.591 | 7.102 | 61.119 | 1.00 | 88.13 | AAAA | C |
| ATOH | 4504 | C2 | IAG | 461 | 59.964 | 7.338 | 59.697 | 1.00 | 91.94 | AAAA | C |
| ATOH | 4506 | HC | IAG | 461 | 58.739 | 7.699 | 58.920 | 1.00 | 92.72 | AAAA | H |
| ATOH | 4508 | C7 | IAG | 461 | 58.400 | 9.020 | 58.999 | 1.00 | 96.97 | AAAA | C |
| ATOH | 4509 | OT | IAG | 461 | 59.879 | 9.774 | 59.726 | 1.00 | 98.62 | AAAA | O |
| ATOH | 4530 | C8 | IAG | 461 | 57.323 | 9.390 | 58.043 | 1.00 | 100.60 | AAAA | C |
| ATOH | 4534 | C3 | IAG | 461 | 60.725 | 6.225 | 59.085 | 1.00 | 94.77 | AAAA | C |
| ATOH | 4536 | C3 | IAG | 461 | 61.417 | 6.725 | 57.930 | 1.00 | 99.51 | AAAA | O |
| ATOH | 4539 | C4 | IAG | 461 | 61.873 | 5.869 | 60.064 | 1.00 | 96.01 | AAAA | C |
| ATOH | 4540 | O4 | IAG | 461 | 62.661 | 4.921 | 59.484 | 1.00 | 99.20 | AAAA | O |
| ATOH | 4543 | C5 | IAG | 461 | 61.359 | 5.529 | 61.474 | 1.00 | 95.13 | AAAA | C |
| ATOH | 4545 | C6 | IAG | 461 | 62.465 | 5.321 | 62.495 | 1.00 | 93.66 | AAAA | C |
| ATOH | 4548 | O6 | IAG | 461 | 62.745 | 6.364 | 63.354 | 1.00 | 92.13 | AAAA | O |
| ATOH | 4544 | C5 | IAG | 461 | 60.625 | 6.549 | 61.949 | 1.00 | 91.92 | AAAA | O |
| ATOH | 4550 | T1 | IAG | 463 | 33.054 | 15.249 | 73.938 | 1.00 | 43.58 | AAAA | C |
| ATOH | 4550 | C2 | IAG | 463 | 31.644 | 15.292 | 73.412 | 1.00 | 43.62 | AAAA | C |
| ATOH | 4554 | HC | IAG | 463 | 30.709 | 14.527 | 72.541 | 1.00 | 42.15 | AAAA | N |
| ATOH | 4556 | C7 | IAG | 463 | 29.912 | 13.584 | 73.099 | 1.00 | 40.84 | AAAA | C |
| ATOH | 4557 | OT | IAG | 463 | 29.929 | 13.406 | 74.222 | 1.00 | 40.10 | AAAA | O |
| ATOH | 4558 | C8 | IAG | 463 | 28.975 | 12.694 | 72.394 | 1.00 | 35.47 | AAAA | C |
| ATOH | 4562 | C3 | IAG | 463 | 31.150 | 16.675 | 73.448 | 1.00 | 45.40 | AAAA | C |
| ATOH | 4564 | O3 | IAG | 463 | 29.979 | 16.555 | 74.196 | 1.00 | 45.99 | AAAA | O |
| ATOH | 4566 | C4 | IAG | 463 | 32.117 | 17.617 | 74.171 | 1.00 | 50.36 | AAAA | C |
| ATOH | 4568 | O4 | IAG | 463 | 31.596 | 18.919 | 73.891 | 1.00 | 53.97 | AAAA | O |
| ATOH | 4569 | C5 | IAG | 463 | 33.589 | 17.477 | 73.725 | 1.00 | 48.50 | AAAA | C |
| ATOH | 4572 | C6 | IAG | 463 | 34.490 | 17.996 | 74.742 | 1.00 | 49.34 | AAAA | C |
| ATOH | 4575 | O6 | IAG | 463 | 34.906 | 18.739 | 75.671 | 1.00 | 57.11 | AAAA | O |
| ATOH | 4571 | O5 | IAG | 463 | 33.942 | 16.120 | 73.583 | 1.00 | 48.58 | AAAA | O |
| ATOH | 4576 | C1 | FUC | 464 | 34.544 | 19.954 | 76.083 | 1.00 | 81.45 | AAAA | C |
| ATOH | 4578 | C2 | FUC | 464 | 35.179 | 21.173 | 75.463 | 1.00 | 86.35 | AAAA | C |
| ATOH | 4579 | O2 | FUC | 464 | 35.153 | 21.169 | 74.021 | 1.00 | 92.94 | AAAA | O |
| ATOH | 4582 | C3 | FUC | 464 | 34.252 | 22.284 | 75.945 | 1.00 | 86.79 | AAAA | C |
| ATOH | 4584 | O3 | FUC | 464 | 34.691 | 23.613 | 75.596 | 1.00 | 87.83 | AAAA | O |
| ATOH | 4586 | C4 | FUC | 464 | 33.871 | 22.274 | 77.412 | 1.00 | 86.67 | AAAA | C |
| ATOH | 4588 | O4 | FUC | 464 | 34.598 | 23.297 | 78.115 | 1.00 | 87.06 | AAAA | O |
| ATOH | 4590 | C5 | FUC | 464 | 33.921 | 20.894 | 78.040 | 1.00 | 85.85 | AAAA | C |
| ATOH | 4593 | C6 | FUC | 464 | 34.279 | 20.768 | 79.512 | 1.00 | 83.37 | AAAA | C |
| ATOH | 4592 | C5 | FUC | 464 | 35.042 | 20.150 | 77.425 | 1.00 | 82.43 | AAAA | O |
| ATOH | 4597 | C1 | IAG | 465 | 31.575 | 19.813 | 74.940 | 1.00 | 64.68 | AAAA | C |
| ATOH | 4599 | C2 | IAG | 465 | 31.267 | 21.207 | 74.437 | 1.00 | 69.57 | AAAA | C |
| ATOH | 4601 | HC | IAG | 465 | 32.480 | 21.642 | 73.690 | 1.00 | 71.25 | AAAA | N |
| ATOH | 4603 | C7 | IAG | 465 | 32.401 | 21.953 | 72.381 | 1.00 | 73.86 | AAAA | C |
| ATOH | 4604 | O7 | IAG | 465 | 31.373 | 21.835 | 71.881 | 1.00 | 74.80 | AAAA | O |
| ATOH | 4605 | C8 | IAG | 465 | 33.679 | 22.401 | 71.787 | 1.00 | 76.00 | AAAA | C |
| ATOH | 4609 | C3 | IAG | 465 | 31.050 | 22.214 | 75.546 | 1.00 | 72.71 | AAAA | C |
| ATOH | 4611 | O3 | IAG | 465 | 30.713 | 23.517 | 75.108 | 1.00 | 71.03 | AAAA | O |
| ATOH | 4613 | C4 | IAG | 465 | 30.035 | 21.654 | 76.560 | 1.00 | 75.71 | AAAA | C |
| ATOH | 4615 | O4 | IAG | 465 | 29.993 | 22.409 | 77.793 | 1.00 | 76.79 | AAAA | O |
| ATOH | 4617 | C5 | IAG | 465 | 30.498 | 20.238 | 76.977 | 1.00 | 75.45 | AAAA | C |
| ATOH | 4620 | C6 | IAG | 465 | 29.461 | 19.647 | 77.930 | 1.00 | 75.64 | AAAA | C |

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|------|------|----|-----|-----|--------|--------|--------|------|--------|------|---|
| ATOH | 4604 | 06 | IAG | 465 | 28.385 | 19.238 | 77.142 | 1.00 | 76.25 | AAAA | O |
| ATOH | 4619 | 05 | IAG | 465 | 30.514 | 19.425 | 75.807 | 1.00 | 71.44 | AAAA | O |
| ATOH | 4625 | 01 | IAG | 467 | 49.927 | 11.058 | 87.926 | 1.00 | 96.51 | AAAA | C |
| ATOH | 4627 | 02 | IAG | 467 | 50.538 | 11.751 | 89.100 | 1.00 | 99.92 | AAAA | C |
| ATOH | 4629 | 02 | IAG | 467 | 49.662 | 12.898 | 89.458 | 1.00 | 101.79 | AAAA | H |
| ATOH | 4631 | 07 | IAG | 467 | 49.299 | 13.021 | 90.759 | 1.00 | 103.63 | AAAA | C |
| ATOH | 4632 | 07 | IAG | 467 | 49.541 | 12.267 | 91.586 | 1.00 | 105.48 | AAAA | O |
| ATOH | 4633 | 08 | IAG | 467 | 48.526 | 14.239 | 91.102 | 1.00 | 105.02 | AAAA | C |
| ATOH | 4637 | 03 | IAG | 467 | 51.967 | 12.134 | 88.802 | 1.00 | 101.03 | AAAA | C |
| ATOH | 4639 | 03 | IAG | 467 | 52.535 | 12.761 | 89.949 | 1.00 | 100.89 | AAAA | O |
| ATOH | 4641 | 04 | IAG | 467 | 52.643 | 10.771 | 88.506 | 1.00 | 101.15 | AAAA | C |
| ATOH | 4643 | 04 | IAG | 467 | 54.067 | 10.834 | 88.441 | 1.00 | 101.35 | AAAA | O |
| ATOH | 4645 | 05 | IAG | 467 | 52.039 | 10.160 | 87.218 | 1.00 | 100.16 | AAAA | C |
| ATOH | 4648 | 06 | IAG | 467 | 52.746 | 8.852 | 86.934 | 1.00 | 99.75 | AAAA | C |
| ATOH | 4651 | 06 | IAG | 467 | 52.088 | 7.704 | 87.302 | 1.00 | 101.54 | AAAA | O |
| ATOH | 4647 | 05 | IAG | 467 | 50.671 | 9.918 | 87.503 | 1.00 | 98.59 | AAAA | O |
| ATOH | 4653 | 01 | IAG | 469 | 55.375 | 46.143 | 66.863 | 1.00 | 48.45 | AAAA | C |
| ATOH | 4655 | 02 | IAG | 469 | 56.601 | 46.993 | 66.861 | 1.00 | 50.42 | AAAA | C |
| ATOH | 4657 | 02 | IAG | 469 | 57.106 | 47.015 | 65.451 | 1.00 | 51.50 | AAAA | H |
| ATOH | 4659 | 07 | IAG | 469 | 57.235 | 48.143 | 64.746 | 1.00 | 48.88 | AAAA | C |
| ATOH | 4660 | 07 | IAG | 469 | 56.849 | 49.101 | 65.234 | 1.00 | 55.62 | AAAA | O |
| ATOH | 4661 | 08 | IAG | 469 | 57.838 | 48.134 | 63.394 | 1.00 | 43.70 | AAAA | C |
| ATOH | 4665 | 03 | IAG | 469 | 57.608 | 46.491 | 67.844 | 1.00 | 49.62 | AAAA | C |
| ATOH | 4667 | 03 | IAG | 469 | 58.640 | 47.461 | 68.031 | 1.00 | 47.76 | AAAA | O |
| ATOH | 4669 | 04 | IAG | 469 | 56.843 | 45.263 | 69.172 | 1.00 | 48.47 | AAAA | C |
| ATOH | 4671 | 04 | IAG | 469 | 57.826 | 45.800 | 70.134 | 1.00 | 50.06 | AAAA | O |
| ATOH | 4672 | 05 | IAG | 469 | 55.847 | 45.130 | 68.959 | 1.00 | 50.81 | AAAA | C |
| ATOH | 4675 | 06 | IAG | 469 | 55.190 | 44.720 | 70.239 | 1.00 | 53.92 | AAAA | C |
| ATOH | 4678 | 06 | IAG | 469 | 54.829 | 45.551 | 71.193 | 1.00 | 56.25 | AAAA | O |
| ATOH | 4674 | 05 | IAG | 469 | 54.914 | 45.599 | 68.043 | 1.00 | 55.45 | AAAA | O |
| ATOH | 4679 | 01 | FUC | 470 | 53.830 | 46.395 | 71.203 | 1.00 | 61.17 | AAAA | C |
| ATOH | 4681 | 02 | FUC | 470 | 53.642 | 47.121 | 72.534 | 1.00 | 59.23 | AAAA | C |
| ATOH | 4682 | 02 | FUC | 470 | 54.861 | 46.876 | 73.241 | 1.00 | 55.14 | AAAA | O |
| ATOH | 4685 | 03 | FUC | 470 | 53.421 | 48.429 | 71.757 | 1.00 | 58.39 | AAAA | C |
| ATOH | 4687 | 03 | FUC | 470 | 53.381 | 49.515 | 72.637 | 1.00 | 56.30 | AAAA | O |
| ATOH | 4689 | 04 | FUC | 470 | 52.245 | 48.255 | 70.809 | 1.00 | 61.24 | AAAA | C |
| ATOH | 4691 | 04 | FUC | 470 | 51.061 | 47.904 | 71.544 | 1.00 | 63.74 | AAAA | O |
| ATOH | 4693 | 05 | FUC | 470 | 52.455 | 47.086 | 69.828 | 1.00 | 62.20 | AAAA | C |
| ATOH | 4696 | 06 | FUC | 470 | 51.462 | 46.723 | 68.784 | 1.00 | 59.15 | | |

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|------|------|----|-----|-----|--------|--------|--------|------------|------|---|
| ATOM | 4771 | 01 | SUL | 493 | 38.452 | -7.921 | 66.345 | 1.00112.65 | DDDD | O |
| ATOM | 4772 | 02 | SUL | 493 | 37.611 | -7.873 | 64.020 | 1.00110.21 | DDDD | O |
| ATOM | 4773 | 03 | SUL | 493 | 36.533 | -6.555 | 65.856 | 1.00109.93 | DDDD | O |
| ATOM | 4774 | 04 | SUL | 493 | 36.333 | -8.978 | 65.639 | 1.00107.58 | DDDD | O |
| ATOM | 4775 | S | SUL | 494 | 56.567 | 19.753 | 66.302 | 1.00109.81 | DDDD | S |
| ATOM | 4776 | 01 | SUL | 494 | 56.597 | 19.128 | 67.659 | 1.00107.98 | DDDD | O |
| ATOM | 4777 | 02 | SUL | 494 | 57.964 | 20.027 | 65.795 | 1.00112.59 | DDDD | O |
| ATOM | 4778 | 03 | SUL | 494 | 55.749 | 21.006 | 66.267 | 1.00111.35 | DDDD | O |
| ATOM | 4779 | 04 | SUL | 494 | 55.886 | 18.792 | 65.379 | 1.00109.86 | DDDD | O |
| ATOM | 4780 | S | SUL | 495 | 34.533 | 11.240 | 75.722 | 1.00114.67 | DDDD | S |
| ATOM | 4781 | 01 | SUL | 495 | 35.274 | 12.213 | 76.595 | 1.00111.38 | DDDD | O |
| ATOM | 4782 | 02 | SUL | 495 | 35.476 | 10.329 | 74.974 | 1.00113.60 | DDDD | O |
| ATOM | 4783 | 03 | SUL | 495 | 33.552 | 11.860 | 74.748 | 1.00112.77 | DDDD | O |
| ATOM | 4784 | 04 | SUL | 495 | 33.773 | 10.278 | 76.604 | 1.00113.18 | DDDD | O |
| ATOM | 4785 | S | SUL | 496 | 35.466 | 24.844 | 59.093 | 1.00 50.73 | DDDD | S |
| ATOM | 4786 | 01 | SUL | 496 | 35.613 | 24.843 | 60.607 | 1.00 62.59 | DDDD | O |
| ATOM | 4787 | 02 | SUL | 496 | 36.002 | 23.581 | 58.571 | 1.00 48.59 | DDDD | O |
| ATOM | 4788 | 03 | SUL | 496 | 35.880 | 26.084 | 58.455 | 1.00 56.74 | DDDD | O |
| ATOM | 4789 | 04 | SUL | 496 | 33.958 | 24.953 | 59.034 | 1.00 59.34 | DDDD | O |
| ATOM | 4790 | S | SUL | 497 | 47.653 | -2.303 | 70.199 | 1.00 68.98 | DDDD | S |
| ATOM | 4791 | 01 | SUL | 497 | 47.849 | -1.058 | 70.996 | 1.00 68.52 | DDDD | O |
| ATOM | 4792 | 02 | SUL | 497 | 48.594 | -2.509 | 69.072 | 1.00 70.94 | DDDD | O |
| ATOM | 4793 | 03 | SUL | 497 | 46.187 | -2.393 | 69.810 | 1.00 73.47 | DDDD | O |
| ATOM | 4794 | 04 | SUL | 497 | 47.799 | -3.446 | 71.129 | 1.00 71.33 | DDDD | O |
| ATOM | 4795 | S | SUL | 498 | 56.527 | 35.758 | 75.513 | 1.00 71.48 | DDDD | S |
| ATOM | 4796 | 01 | SUL | 498 | 55.870 | 35.013 | 76.621 | 1.00 72.97 | DDDD | O |
| ATOM | 4797 | 02 | SUL | 498 | 57.759 | 34.996 | 75.167 | 1.00 69.11 | DDDD | O |
| ATOM | 4798 | 03 | SUL | 498 | 56.619 | 37.237 | 75.785 | 1.00 72.45 | DDDD | O |
| ATOM | 4799 | 04 | SUL | 498 | 55.623 | 35.809 | 74.330 | 1.00 72.74 | DDDD | O |
| ATOM | 4800 | S | SUL | 499 | 40.639 | 27.365 | 69.499 | 1.00 74.04 | DDDD | S |
| ATOM | 4801 | 01 | SUL | 499 | 40.218 | 26.039 | 70.045 | 1.00 76.00 | DDDD | O |
| ATOM | 4802 | 02 | SUL | 499 | 42.089 | 27.608 | 69.835 | 1.00 75.15 | DDDD | O |
| ATOM | 4803 | 03 | SUL | 499 | 39.823 | 28.467 | 70.098 | 1.00 77.27 | DDDD | O |
| ATOM | 4804 | 04 | SUL | 499 | 40.424 | 27.245 | 68.018 | 1.00 75.70 | DDDD | O |
| ATOM | 4805 | S | SUL | 500 | 44.996 | 53.229 | 20.568 | 1.00 83.89 | DDDD | S |
| ATOM | 4806 | 01 | SUL | 500 | 45.080 | 54.400 | 21.461 | 1.00 84.79 | DDDD | O |
| ATOM | 4807 | 02 | SUL | 500 | 46.109 | 52.266 | 20.827 | 1.00 90.38 | DDDD | O |
| ATOM | 4808 | 03 | SUL | 500 | 45.032 | 53.674 | 19.135 | 1.00 92.23 | DDDD | O |
| ATOM | 4809 | 04 | SUL | 500 | 43.762 | 52.396 | 20.723 | 1.00 91.61 | DDDD | O |
| ATOM | 4810 | OW | WAT | 501 | 29.970 | 6.904 | 77.713 | 1.00 34.84 | DDDD | O |
| ATOM | 4811 | OW | WAT | 502 | 42.522 | 18.998 | 79.232 | 1.00 55.27 | DDDD | O |
| ATOM | 4812 | OW | WAT | 503 | 37.561 | 21.003 | 67.518 | 1.00 41.63 | DDDD | O |
| ATOM | 4813 | OW | WAT | 504 | 50.446 | 5.721 | 63.485 | 1.00 57.37 | DDDD | O |
| ATOM | 4814 | OW | WAT | 505 | 56.668 | 24.854 | 72.729 | 1.00 57.34 | DDDD | O |
| ATOM | 4815 | OW | WAT | 506 | 50.605 | 57.695 | 22.727 | 1.00 54.26 | DDDD | O |
| ATOM | 4816 | OW | WAT | 507 | 55.123 | 37.781 | 61.204 | 1.00 43.71 | DDDD | O |
| ATOM | 4817 | OW | WAT | 508 | 17.414 | -9.070 | 74.793 | 1.00 48.79 | DDDD | O |
| ATOM | 4818 | OW | WAT | 509 | 44.263 | 20.885 | 63.811 | 1.00 29.64 | DDDD | O |
| ATOM | 4819 | OW | WAT | 510 | 45.085 | 19.708 | 94.433 | 1.00 49.09 | DDDD | O |
| ATOM | 4820 | OW | WAT | 511 | 33.537 | 1.927 | 71.115 | 1.00 60.39 | DDDD | O |
| ATOM | 4821 | OW | WAT | 512 | 19.279 | 4.902 | 75.254 | 1.00 55.23 | DDDD | O |
| ATOM | 4822 | OW | WAT | 513 | 11.502 | -0.835 | 69.996 | 1.00 57.51 | DDDD | O |
| ATOM | 4823 | OW | WAT | 514 | 24.591 | 17.207 | 56.665 | 1.00 56.36 | DDDD | O |
| ATOM | 4824 | OW | WAT | 515 | 56.947 | 34.914 | 62.552 | 1.00 36.47 | DDDD | O |
| ATOM | 4825 | OW | WAT | 516 | 58.092 | 39.983 | 66.234 | 1.00 30.34 | DDDD | O |
| ATOM | 4826 | OW | WAT | 517 | 48.308 | 40.726 | 56.768 | 1.00 81.69 | DDDD | O |
| ATOM | 4827 | OW | WAT | 518 | 25.776 | 2.355 | 85.630 | 1.00 66.34 | DDDD | O |
| ATOM | 4828 | OW | WAT | 519 | 30.644 | 68.108 | 30.765 | 1.00 82.28 | DDDD | O |
| ATOM | 4829 | OW | WAT | 520 | 38.739 | 54.257 | 43.611 | 1.00 43.41 | DDDD | O |
| ATOM | 4830 | OW | WAT | 521 | 22.886 | 4.470 | 64.871 | 1.00 48.71 | DDDD | O |
| ATOM | 4831 | OW | WAT | 522 | 30.938 | 50.249 | 19.364 | 1.00 54.00 | DDDD | O |
| ATOM | 4832 | OW | WAT | 523 | 32.413 | 9.061 | 42.441 | 1.00 44.45 | DDDD | O |
| ATOM | 4833 | OW | WAT | 524 | 41.019 | 42.560 | 55.653 | 1.00 43.40 | DDDD | O |
| ATOM | 4834 | OW | WAT | 525 | 54.268 | 51.393 | 37.513 | 1.00 55.10 | DDDD | O |
| ATOM | 4835 | OW | WAT | 526 | 37.130 | 13.599 | 81.397 | 1.00 46.49 | DDDD | O |
| ATOM | 4836 | OW | WAT | 527 | 42.585 | 10.244 | 84.472 | 1.00 35.95 | DDDD | O |
| ATOM | 4837 | OW | WAT | 528 | 43.661 | 61.633 | 18.450 | 1.00 41.05 | DDDD | O |
| ATOM | 4838 | OW | WAT | 529 | 27.980 | 19.862 | 53.348 | 1.00 54.59 | DDDD | O |
| ATOM | 4839 | OW | WAT | 530 | 59.527 | 38.520 | 64.116 | 1.00 37.96 | DDDD | O |
| ATOM | 4840 | OW | WAT | 531 | 22.451 | 1.046 | 57.437 | 1.00 59.31 | DDDD | O |
| ATOM | 4841 | OW | WAT | 532 | 30.380 | 16.123 | 70.205 | 1.00 40.39 | DDDD | O |
| ATOM | 4842 | OW | WAT | 533 | 46.835 | 27.888 | 65.854 | 1.00 52.34 | DDDD | O |
| ATOM | 4843 | OW | WAT | 534 | 39.446 | 49.001 | 45.379 | 1.00 46.05 | DDDD | O |
| ATOM | 4844 | OW | WAT | 535 | 46.992 | 51.272 | 50.722 | 1.00 52.62 | DDDD | O |
| ATOM | 4845 | OW | WAT | 536 | 44.263 | 18.776 | 73.017 | 1.00 40.61 | DDDD | O |
| ATOM | 4846 | OW | WAT | 537 | 33.670 | 59.861 | 20.848 | 1.00 51.56 | DDDD | O |
| ATOM | 4847 | OW | WAT | 538 | 52.469 | 21.639 | 73.804 | 1.00 61.98 | DDDD | O |
| ATOM | 4848 | OW | WAT | 539 | 49.985 | 44.871 | 37.324 | 1.00 45.45 | DDDD | O |
| ATOM | 4849 | OW | WAT | 540 | 24.074 | -1.791 | 60.077 | 1.00 40.40 | DDDD | O |
| ATOM | 4850 | OW | WAT | 541 | 35.207 | 0.714 | 79.039 | 1.00 51.34 | DDDD | O |
| ATOM | 4851 | OW | WAT | 542 | 31.231 | -1.176 | 62.362 | 1.00 48.33 | DDDD | O |
| ATOM | 4852 | OW | WAT | 543 | 41.726 | -5.156 | 55.290 | 1.00 60.67 | DDDD | O |
| ATOM | 4853 | OW | WAT | 544 | 48.564 | 37.335 | 72.612 | 1.00 71.69 | DDDD | O |
| ATOM | 4854 | OW | WAT | 545 | 49.501 | 40.030 | 67.582 | 1.00 44.88 | DDDD | O |
| ATOM | 4855 | OW | WAT | 546 | 54.851 | 7.987 | 60.018 | 1.00 49.91 | DDDD | O |

| Face 1 | Cleft 1 | Face 2 | Cleft 2 | Face 3 |
|--|---------|--------------------------|---------|-----------------------|
| (12D) 11N 10R 8D (6G) 5P | | 259E 261S 262D | | |
| (35S) 33L 32L 30H 28Y (27G) 26E 255I | | 256L 263S 264E | | 310T 312D 335R |
| (61A) 59R 58F 56L 54Y 53E 242E 241F (274M) | | 266F 275Q 276E 282I 300K | | (316S) 313S 336R |
| 91E 90F 82F (88V) 83Y 80K 79W | | 272E 279S 298C | | 315T 314V (344V) 338N |
| 115K 114E 112R 85Y 84N 108R | | 240R (280G) 270D | | 346Q 343E |
| (140V) 138Y | | | | |

Figure 2

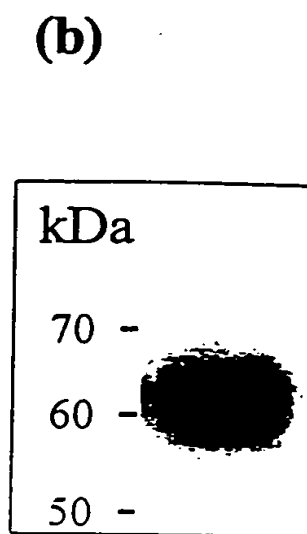
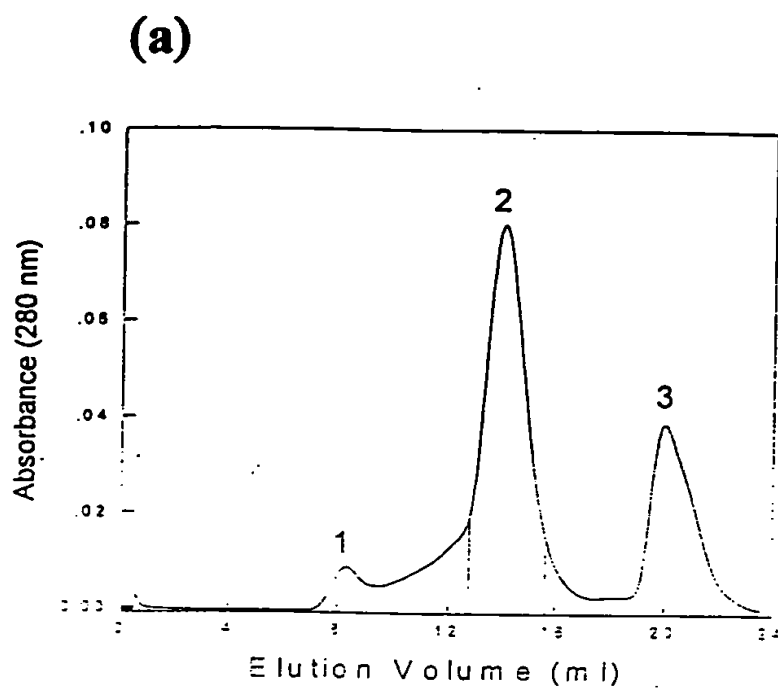


Figure 3

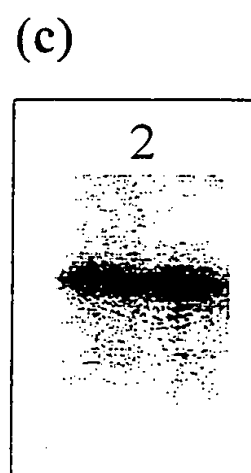
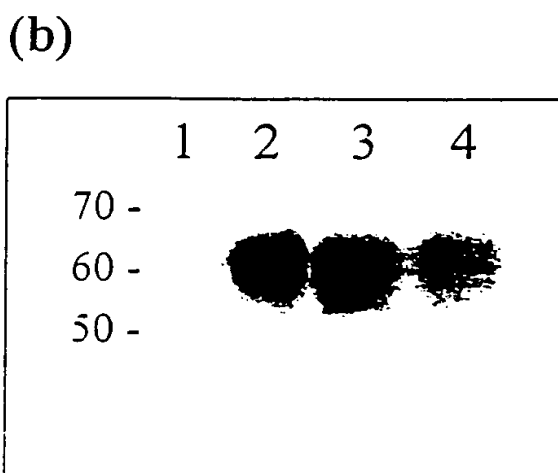
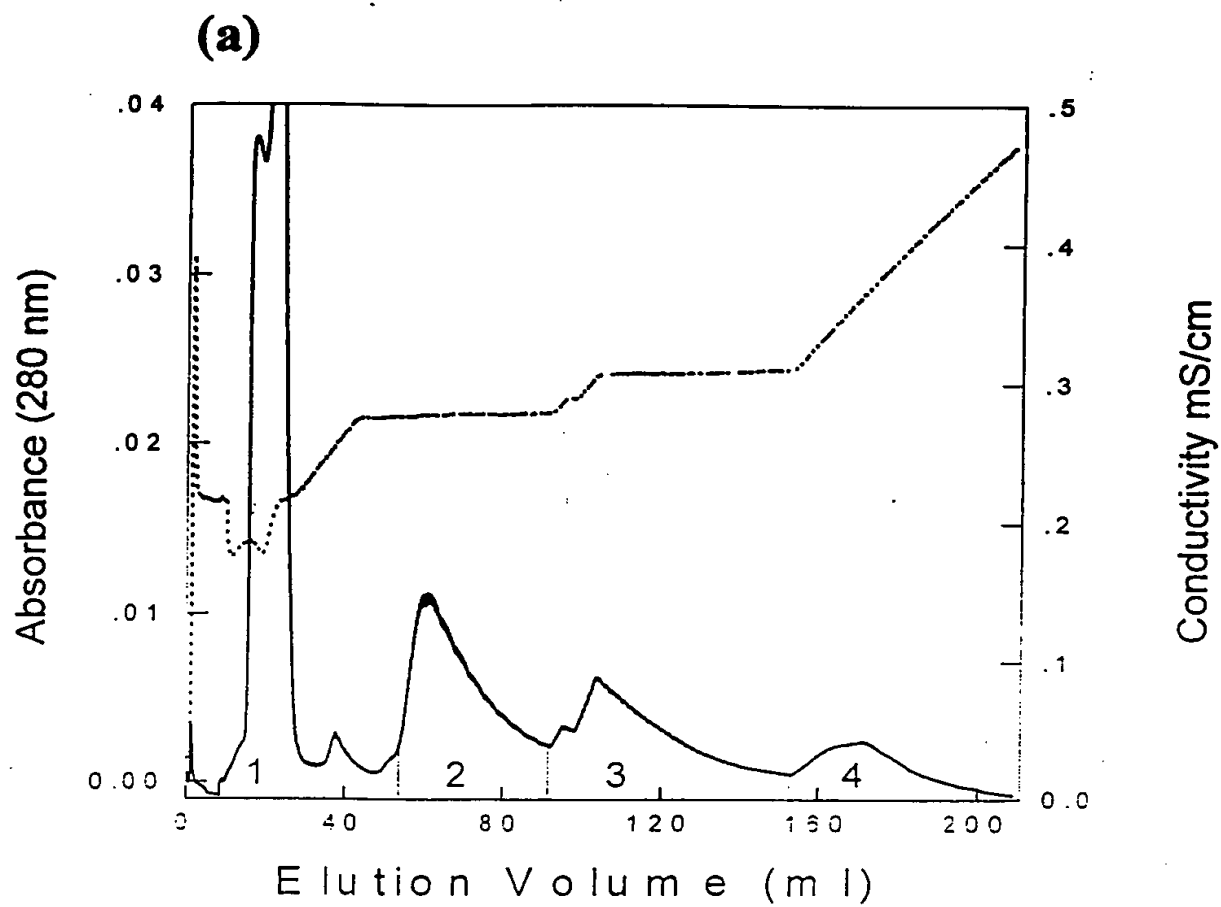


Figure 4

Figure 5

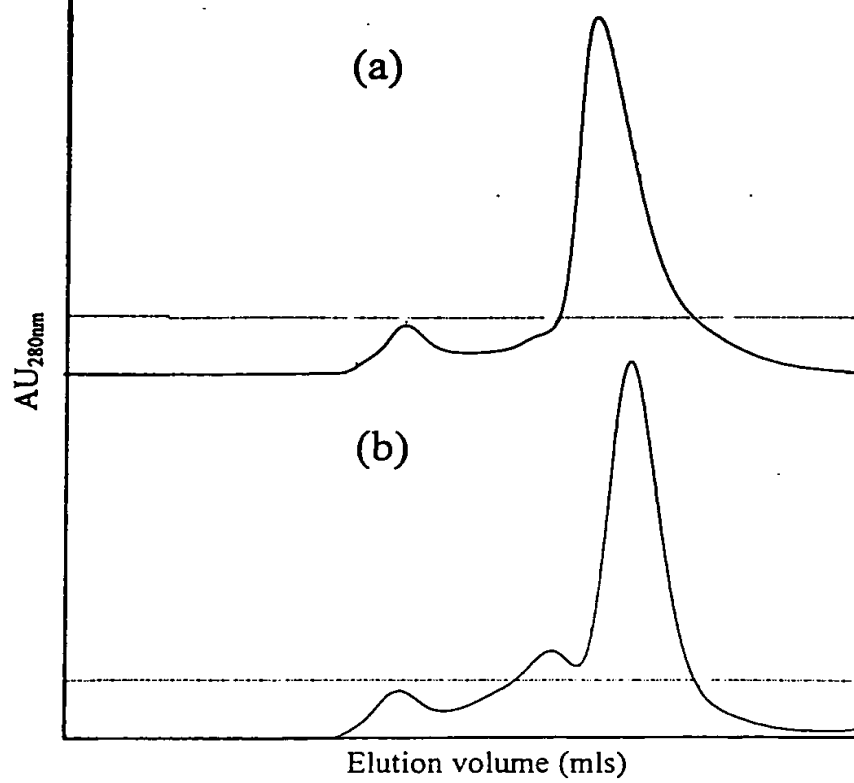
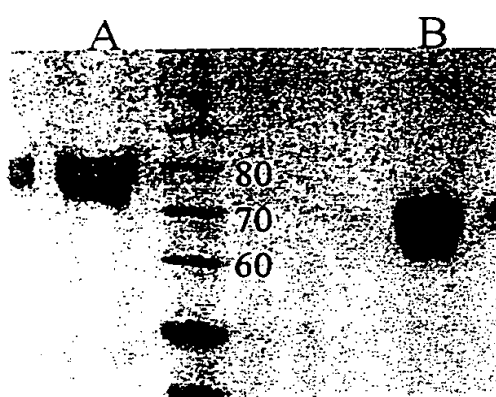
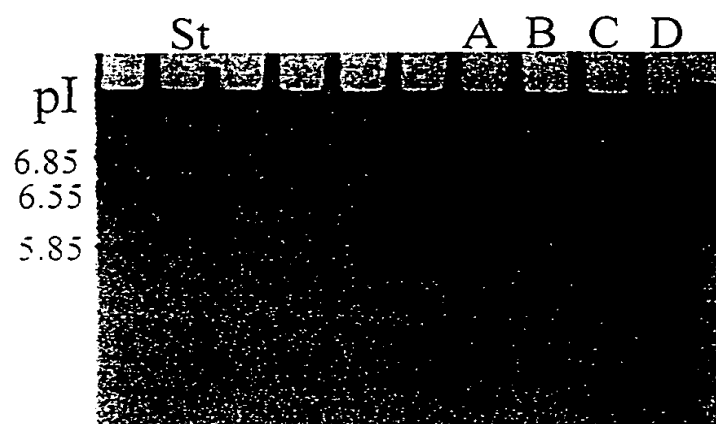


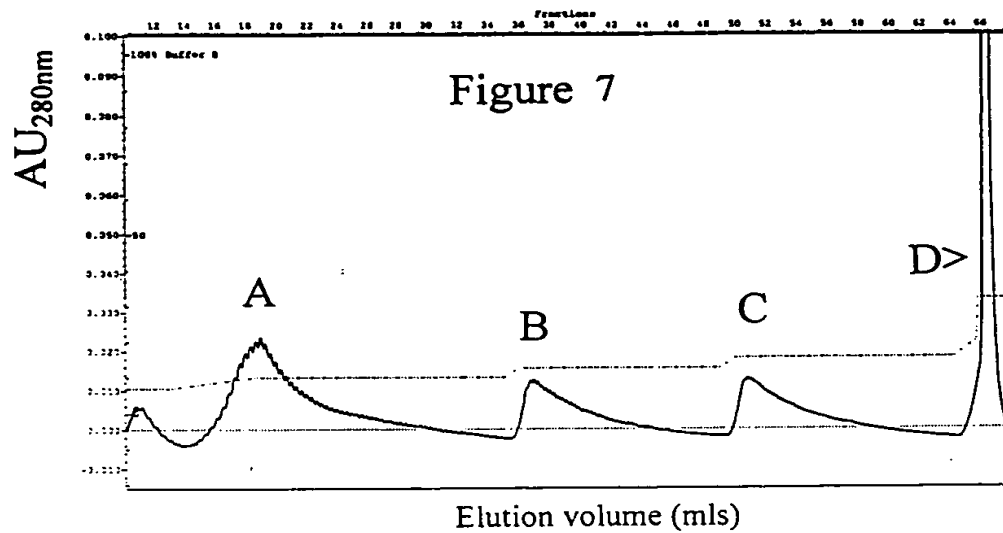
Figure 6

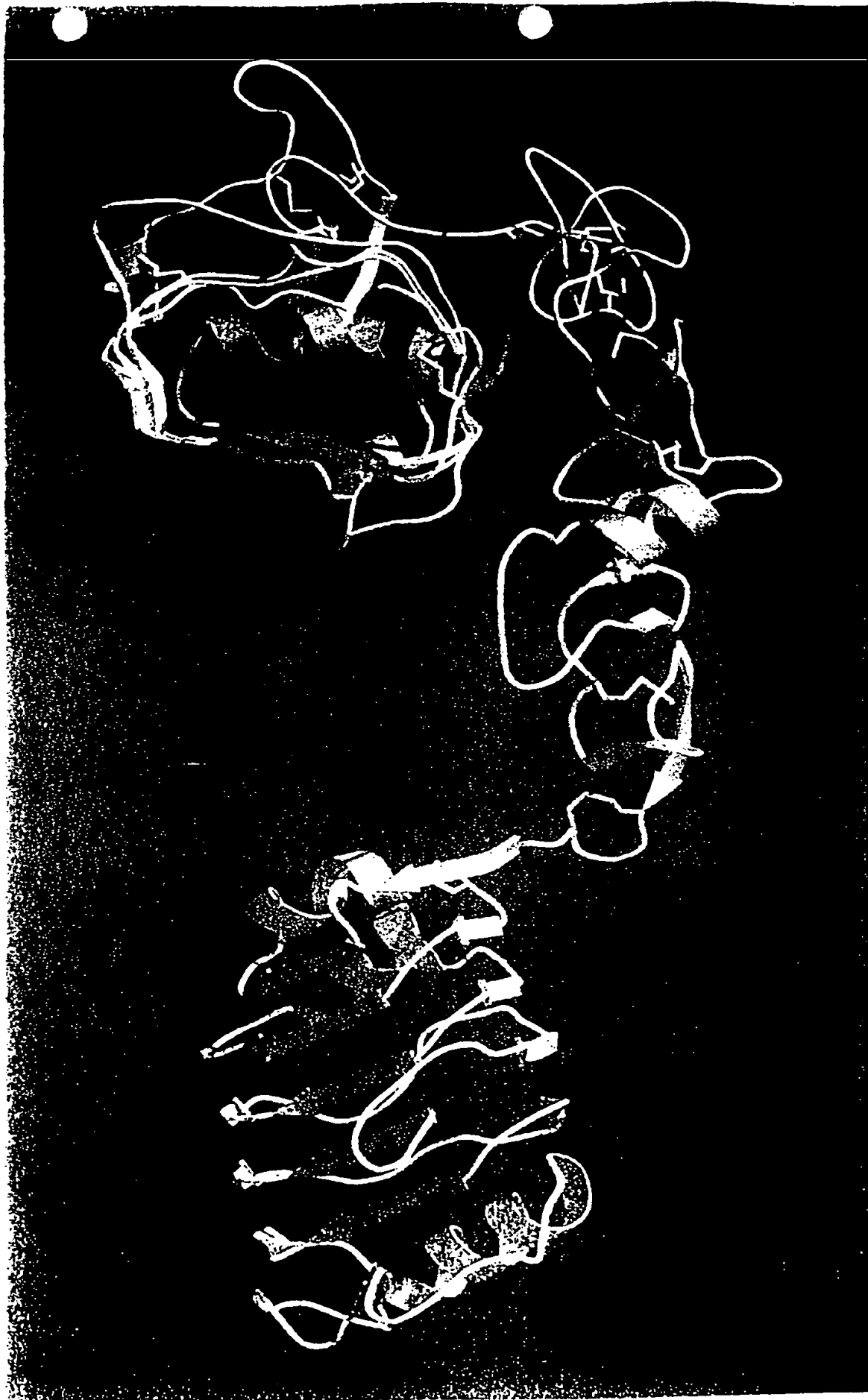
(a) SDS PAGE



(b) IEF pH3-7







| | | | | | | | | | |
|----------|-----|-----------|-----------------|-----------------|---------------|---------------|---------------|-----------|----|
| IGF1R L1 | I | E I C G P | G I D I R N | D Y Q L K R | L E N C T V I | E G Y L H I | L L I S K A | E D Y R S | 42 |
| IR L1 | I | G E V C P | G M D I R N | N L T R L E | E N C S V I | L L M F K T | R P E D F R D | 48 | |
| EGFR L1 | I | L E E K | G T S N K L (9) | L S L Q R M F | E N C E V V | L L Y V Q R N | Y D | 51 | |
| EGFR L2 | 311 | K V C N | G I G I G E (7) | N A T N I K H F | E N C T S I | L L P V A G N | P P L D P Q E | 367 | |
| IR L2 | 310 | K V C H L | L E G E K T I D | S V T S A Q M L | E N C T V I | L L I R G G N | N I A A E L E | 355 | |
| IGF1R L2 | 300 | K V C E | E E K K T I D | S V T S A Q M L | E N C T V I | L L I R G G N | N I A A E L E | 345 | |

[illegible][illegible]

IGF1R 150 D L C P G T M E E K P M C E K T T I N N E Y N Y R C W T T N R C K K 183
 IR 157 D I C P G T A K G K T N C P A T V I N G Q F V E R C W T T S H C K K 190
 EGFR D2 165 K C C D P L C S P L C S P E G C W G A G F E N C K L T K I 189
 EGFR D4 -480 Q V C H A L C S P L C S P E G C W G A G F E N C K L T K I S C R N E V S R G R E E C V D K 515

Module 1

MCPS T C G K R A C T E N E C C H P E C L G S C S A P D N D T A C V A C R H Y Y A G V C V P A C P P N 237
 VCPT I C K S H G C T A E G L C C H S E C L G N C S Q P D D P T K C C V A C R N F Y Y L D E A T T C V E T C P P P 244
 LCAQQCS GRCRGKSPS D C C H N Q C A A G C T G P R E S D C L C C R K F R D E A T T C V E T C P P P L 243
 CKLLEGEPRFVENSECIQCCHPECLPQAMNI T C T G R G P D N C I Q C A H Y I D G P H C V K T C P A G 575

Module 2

Module 3

Module 4

MLYNPTTYQNDVNP E G K Y S F G T Y R F E G W R C V D R D F C A N I L S A E S S D S E G F V I H D G E C M Q 275
 VMGE NNTLVWKYADAGHV C H L C H P N C T Y G C T G P G L E G C P T A N G R P K L E P S S R N Y V V T D H N K C I P 286
 285 622

Module 5

Module 6

ECPS GF I R N G S Q S M Y C I P C E G P C P 309
 ECPS G Y T M N S S N L L C T P C L G P C P 309
 AC G A D S Y E M E D G V R K C K K C E G P C R 310

Module 7

Module 8

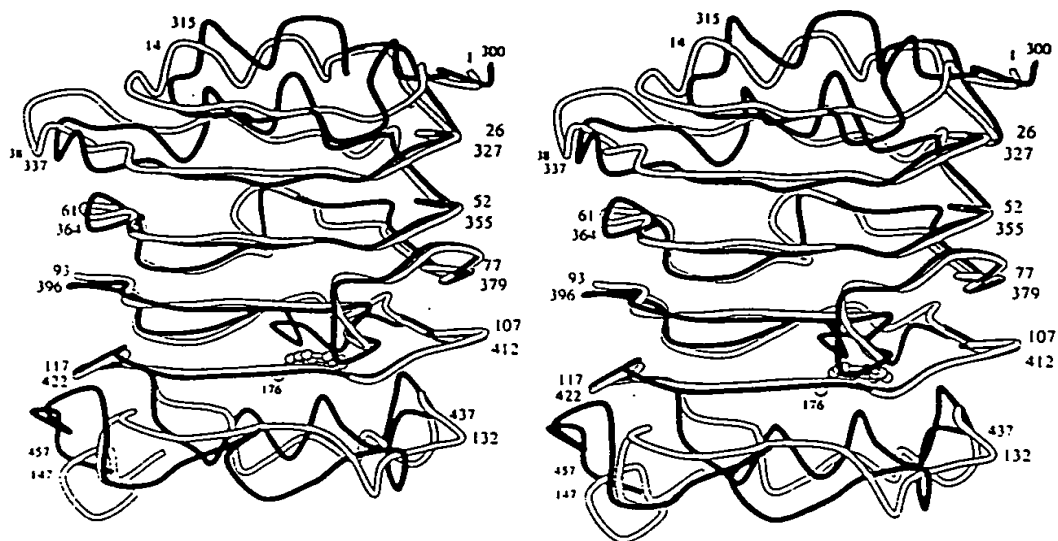


Figure 10

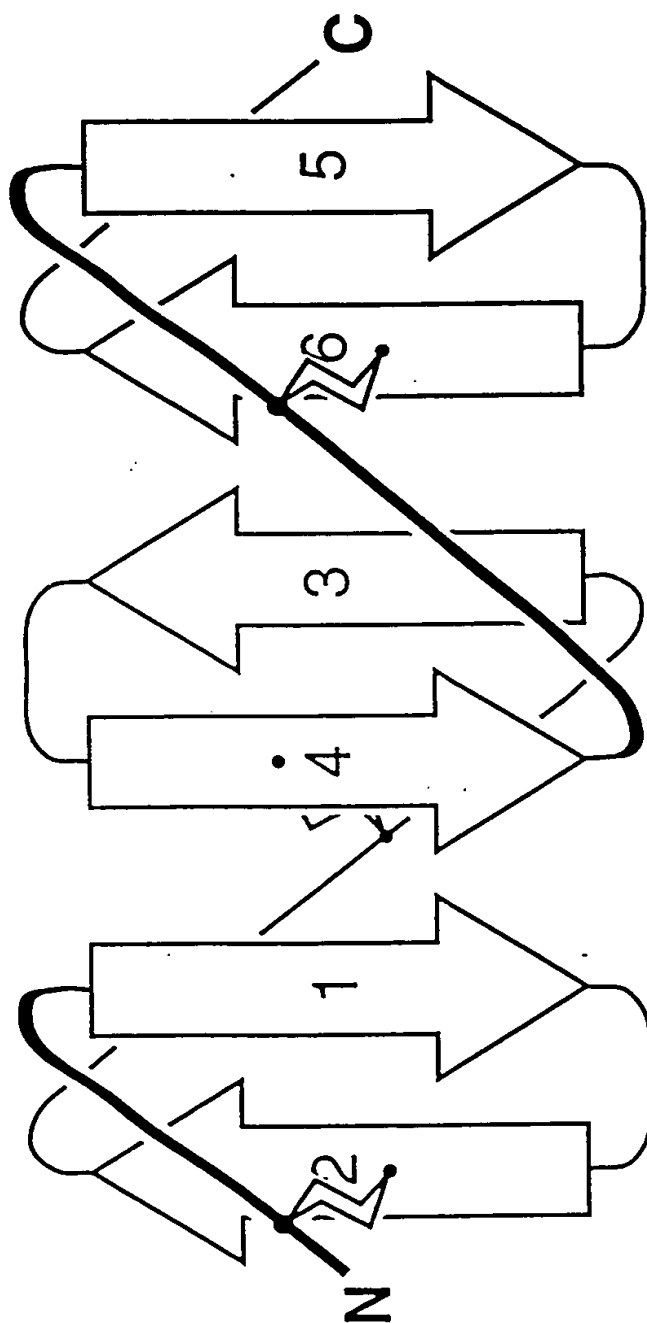


Figure 11

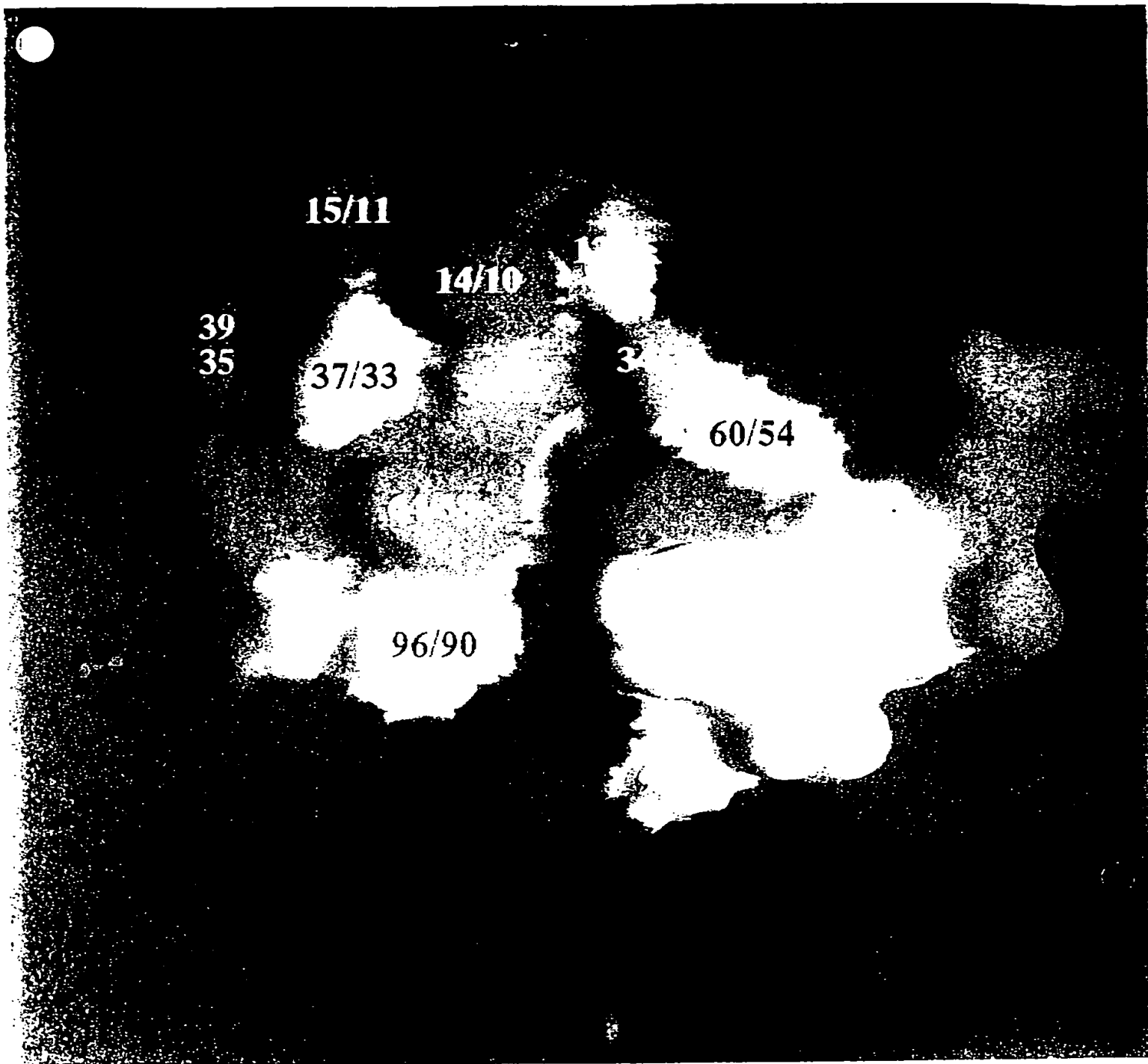


Figure 12

Figure 13: Sequence Alignment of hIGF-1R, hIR and hIRR ectodomains.

Derived by use of the PileUp program in the software package of the Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA.

Symbol Comparison table: GenRunData:PileUpPep.Cmp CompChck: 1254

GapWeight: 3.0
GapLengthWeight: 0.1

| | | | |
|--------------|----------|-------------|--------------|
| Name: Higflr | Len: 972 | Check: 1781 | Weight: 1.00 |
| Name: Hir | Len: 972 | Check: 2986 | Weight: 1.00 |
| Name: Hirr | Len: 972 | Check: 9819 | Weight: 1.00 |


```

      *
Higflr  ....EICGP GIDIRNDYQQ LKRLENCTVI EGYLHILLIS K..AEDYRSY 43
      Hir  HLYPGEVC.P GMDIRNNLTR LHELENCSVI EGYLQILLMF KTRPEDFRDL 49
      Hirr  ....MNV.C.P SLDIRSEVAE LRQLENCSVV EGYLQILLMF TATGEDFRGL 45

      *
Higflr  RFPKLTVITE YLLLFRVAGL ESLGDLFPNL TVIRGWKLFY NYALVIFEMT 93
      Hir  SFPKLIMITD YLLLFRVYGL ESLKDLFPNL TVIRGSRLFF NYALVIFEMV 99
      Hirr  SFPRLTQVTD YLLLFRVYGL ESLRDLFPNL AVIRGTRLFL GYALVIFEMP 95

      *
Higflr  NLKDIGLYNL RNITRGAIRI EKNADLCYLS TVDWSLILDA VSNNYIVGNK 143
      Hir  HLKELGLYNL MNITRGSVRI EKNNELCYLA TIDWSRILDS VEDNYIVLNLK 149
      Hirr  HLRDVALPAL GAVLRGAVRV EKNQELCHLS TIDWGLLQPA PGANHIVGNK 145

      * * * *
Higflr  PPK.ECGDLC PGTMEEEKPM. CEKTTINNEY NYRCWTTNRC QKMCPSTCGK 191
      Hir  DDNEECGDIC PGTAAGKTN. CPATVINGQF VERCWTHSHC QKVCPTICKS 198
      Hirr  LG.EECADV CPGVLGAAGEP CAKTTFSGHT DYRCWTSSHC QRVCPCPHG. 193

      * ** * * *
Higflr  RACTENNECC HPECLGSCSA PDNDTACVAC RHYYYAGVCV PACPPNTYRF 241
      Hir  HGCTAEGGCC HSECLGNCSQ PDDPTKCVAC RNFYLDGRCV ETCPPPPYHF 248
      Hirr  MACTARGECC HTECLGGCSQ PEDPRACVAC RHLVFQGAQL WACPPGTYQY 243

      * * * *
Higflr  EGWRCVDRDF CANILSAES. ...SDSEGFV IHGECMQEC PSGFIRNGSQ 287
      Hir  QDWRVCNFSF QDDLHHKCKN SRRQGCHQYV IHNNKCTPEC PSGYTMNSSN 298
      Hirr  ESWRCVTAER CASLHSPVG. ....RASTFG IHQGSCLAQC PSGFTRNSS. 287

      * * * *
Higflr  SMCIPCEGP CPKVCEEEKK TKTIDSVTSA QMLQGCTIFK GNLLINIRRG 337
      Hir  .LLCTPCLGP CPKVCHLLEG EKTIDSVTSA QELRGCTVIN GSLIINIRGG 347
      Hirr  SIFCHKCEGL CPKECKV..G TKTIDSIQAA QDLVGCTHVE GSLILNLRQG 335

      *
Higflr  NNIASELENF MGLIEVVTGY VKIRSHALV SLSFLKNLRL ILGEEQLEGN 387
      Hir  NNLAEELEAN LGLIEEISGY LKIRRSYALV SLSFFRKLRL IRGETLEIGN 397
      Hirr  YNLEPQLQHS LGLVETITGF LKIKHSFALV SLGFFKNLKL IRGDAMVDGN 385

      *
Higflr  YSFYVLNDQN LQQLWDWDHR NLTIKAGKMY FAFNPKLCVS EIYRMEEVTG 437
      Hir  YSFYALDNQN LRQLWDWSKH NLTITQGKLF FHYNPKLCLS EIHKMEEVSG 447
      Hirr  YTLYVLNDQN LQQLGSWVAA GLTIPVGKIY FAFNPRLCLE HIYRL EEVG 435

      *
Higflr  TKGRQSKGDI NTRNNGERAS CESDV LHFTS TTTSKNRIII TWHRYRPPDY 487
      Hir  TKGRQERNDI ALKTNGDQAS CENEL LKFSY IRTSFDKILL RWEPYWPPDF 497
      Hirr  TRGRQNKAEI NPRTNGDRAA CQTRT LRFVS NVTEADRILL RWERYEPLEA 485
  
```

| | | | | | | |
|----------------|-------------|------------|------------|------------|-------------|-----|
| Higflr | RDLSFTVYY | KEAPFKNVTE | YDQDACGSN | SWNMVDVDLP |PNKDV | 532 |
| Hir | RDLLGFMIFY | KEAPYQNVTE | FDGQDACGSN | SWTVVDIDPP | LRSDNPKSQN | 547 |
| Hirr | RDLLSFIVYY | KESPFONATE | HVGPDACGTQ | SWNLLDVELP | L.....SRTQ | 530 |
| | | | | | | |
| Higflr | EPGILLHGLK | PWTQYAVYVK | AVTLTMVEND | HIRGAKSEIL | YIRTNASVPS | 582 |
| Hir | HPGWLMRGLK | PWTQYAIQVK | TL.VTFSDER | RTYGAKSDII | YVQTDATNPS | 596 |
| Hirr | EPGVTLASLK | PWTQYAVFVR | AITLTTEEDS | PHQGAQSPIV | YLRTLPAAPT | 580 |
| | | | | | | |
| Higflr | IPLDVLSASN | SSSQLIVKWN | PPSLPENGNS | YYIVRWQRQP | QDGYLYRHNY | 632 |
| Hir | VPLDPISVSN | SSSQIILKWK | PPSDPENGNT | HYLVFWERQA | EDSELFELDY | 646 |
| Hirr | VPQDVISTSN | SSSHLLVRWK | PPTQRNGNLT | YYLVWLQRLA | EDGDLYLNDY | 630 |
| | | | | | | |
| Higflr | CSKD.KIPIR | KYADGTIDIE | EVTENPKTEV | CGGEKGPCCA | C...PKTEAE | 678 |
| Hir | CLKGLKLPSR | TWS.PPFESE | DSQKHNOSE. | YEDSAGECCS | C...PKTDSQ | 691 |
| Hirr | CHRGRLRLPTS | N.NDPRFDGE | DGDPEAEME. |SDCCP | CQHPPPGQVL | 673 |
| | | | | | | |
| α-----><-----β | | | | | | |
| Higflr | KQAEKEEAAY | RKVFENFLHN | SIFVPRPERK | RRDVMQVANT | TMSSRSRNTT | 728 |
| Hir | ILKELEESSF | RKTFEDYLHN | VVFVPRPSRK | RRSLGDVGNV | TVAVP...TV | 738 |
| Hirr | PPLAQEASF | QKKFENFLHN | AITIPISPWK | VTSINKSPQR | D.SGRHRRAA | 722 |
| | | | | | | |
| Higflr | AA..DTYNIT | DPEELETEYP | FFESRVDNKE | RTVISNLRPF | TLYRIDIHSC | 776 |
| Hir | AAFPNTSSTS | VPTSPEEHRP | F..EKVVNKE | SLVISGLRHF | TGYRIELQAC | 786 |
| Hirr | GPLRLGGNSS | DFEIQEDKVP |RE | RAVLSGLRHF | TEYRIDIHAC | 764 |
| | | | | | | |
| Higflr | NHEAEKLGCS | ASNFVFARTM | PAEGADDIPG | PVTWEPRPEN | SIFLKWPEPE | 826 |
| Hir | NQDTPEERCS | VAAYVSARTM | PEAKADDIVG | PVTHEIFENN | VVHLMWQEPK | 836 |
| Hirr | NHAAHTVGCS | AATFVFARTM | PHREADGIPG | KVAWEASSKN | SVLLRWLEPP | 814 |
| | | | | | | |
| Higflr | NPNGLILMYE | IKYGS.QVED | QRECVSRQEV | RKYGGAKLNR | LNPNGNYTARI | 875 |
| Hir | EPNGLIVLYE | VSYRRYGDEE | LHLCVSRKHF | ALERGCRLRG | LSPGNYSVRI | 886 |
| Hirr | DPNGLILKYE | IKYRRLGEEA | TVLCVSRLRY | AKFGGVHLAL | LPPGNY SARV | 864 |
| | | | | | | |
| Higflr | QATSLSGNGS | WTDPVFFYVQ | AKTGYENFIH | L | | 906 |
| Hir | RATSLAGNGS | WTEPTYFYVT | DYLDVPSNIA | K | | 917 |
| Hirr | RATSLAGNGS | WTDSVAFYIL | GPEEDAGGL | H | | 895 |

Figure 14: Sequence Alignment of EGFR, ErbB2, ErbB3 and ErbB4 Ectodomains.

[For alignment on the IGF-1R fragment see Fig. 9]

Derived by use of the PileUp program in the software package of the Genetics Computer Group, 575 Science Drive, Madison, Wisconsin, USA.

Symbol comparison table: GenRunData:Pileuppep.Cmp CompCheck: 1254

GapWeight: 3.000
GapLengthWeight: 0.100

| | | | |
|------------|----------|-------------|--------------|
| Name: Erb3 | Len: 649 | Check: 4625 | Weight: 1.00 |
| Name: Erb4 | Len: 649 | Check: 790 | Weight: 1.00 |
| Name: Egfr | Len: 649 | Check: 2381 | Weight: 1.00 |
| Name: Erb2 | Len: 649 | Check: 8174 | Weight: 1.00 |

| | |
|--|-----|
| 1 | 50 |
| Erb3 SEVGNSQAVC PGTNLGLSVT GDAENQYQTL YKLYERCEVV MGNLEIVLTG | |
| Erb4 ...SDSQSVC AGTENKLSSL SDLEQQYRAL RKYYENCEVV MGNLEITSIE | |
| Egfr ...LEEKKVC QGTSNKLTQL GTFEDHFLSL QRMFNNCEVV LGNLEITYVQ | |
| Erb2STQVC TGTDMKLRLP ASPETHLDML RHLYQGCQVV QGNLELTYLP | |
| 51 | 100 |
| Erb3 HNADLSFLQW IREVTGYVLV AMNEFSTLPL PNLRVVRGTQ VYDGKFAIFV | |
| Erb4 HNRDLSFLRS VREVTGYVLV ALNQFRYLPL ENLRIIRGTK LYEDRYALAI | |
| Egfr RNYDLSFLKT IQEVAGYVLI ALNTVERIPL ENLQIIRGNM YYENSYALAV | |
| Erb2 TNASLSFLQD IQEVQGYVLI AHNQVRQVPL QRLRIVRGTO LFEDNYALAV | |
| 101 | 150 |
| Erb3 MLNYN..... TNSSHA LRQLRLTQLT EILSGGVYIE KNDKLCHMDT | |
| Erb4 FLNYR..... KDGNGF LQELGLKNLT EILNGGVYVD QNKFLCYADT | |
| Egfr LSNYD..... ANKT.G LKELPMRNLQ EILHGA VRFS NNPALCNVES | |
| Erb2 LDNGDPLNNT TPVTGASPGG LRELQLRSLT EILKGGVLIQ RNPQLCYQDT | |
| 151 | 200 |
| Erb3 IDWRDIVRDR ...DAEIVVK DNGRSCPPCH EVC.KGRCWG PGSEDCQTLT | |
| Erb4 IHWQDIVRNP WPSNLTIVST NGSSGCGRCH KSC.TGRCWG PTENHCQTLT | |
| Egfr IQWRDIVSSD FLSNMSMDFQ NHLGSCQKCD PSCPNGSCWG AGEENCQKLT | |
| Erb2 ILWKDIFHKV NQLALTIDT NRSRACHPCS PMCKGSRCWG ESSEDCQSLT | |
| 201 | 250 |
| Erb3 KTICAPQCNG HCFGPNPNQC CHDECAGGCS GPQDTCDFAC RHFNDSGACV | |
| Erb4 RTVCAEQCDG RYGPYVSDC CHRECAGGCS GPKDTCDFAC MNFNDSGACV | |
| Egfr KIICAQQCSG RCRGKSPSDC CHNQCAAGCT GPRESDECLVC RKFRDEATCK | |
| Erb2 RTVCAGGC.A RCKGPLPTDC CHEQCAAGCT GPKHSDCLAC LHFNHSGICE | |
| 251 | 300 |
| Erb3 PRCPQPLVYN KLTFOLEPNP HTKYQYGGVC VASCPHNFVV .DQTSVVRAC | |
| Erb4 TQCPQTFVYN PTFQLEHNF NAKYTYGAFV VKKCPHNFVV .DSSSCVRAC | |
| Egfr DTCPPMLLYN PTYQMDVNP EGKYSFGATC VKKCPRNYVV TDHGSCVRAC | |
| Erb2 LHCPALVTYN TDTFESMPNP EGRYTFGASC VTACPYNVLS TDVGSCTLVC | |
| 301 | 350 |
| Erb3 PPDKMEV.DK NGLKMCEPCG GLCPKACEGT GSGSRF..QT VDSSNIDGFV | |
| Erb4 PSSKMEV.EE NGIKMCKPCT DICPKACDGI GTGSLMSAQT VDSSNIDKFI | |
| Egfr GADSYEM.EE DGVRKCKKCE GPCRKVCNGI GIGEFKDSLS INATNIKHFV | |
| Erb2 PLHNQEVTAE DGTQRCEKCS KPCARVCYGL GMEHLREVRA VTSANIQEFA | |
| 351 | 400 |
| Erb3 NCTKILGNLD FLITGLNGDP WHKIPALDPE KLVNFRVTVRE ITGYLNIQSW | |
| Erb4 NCTKINGNLI FLVTGIHGDP YNAIEAIDPE KLVNFRVTVRE ITGFLNIQSW | |
| Egfr NCTSIGDLH ILPVAFRGDS FTHTPPLDPQ ELDILKTVKE ITGFLLIQAW | |
| Erb2 GCKKIFGSLA FLPEFSDGDP ASNTAPLQPE QLQVFETLEE ITGYLYISAW | |
| 401 | 450 |
| Erb3 PPHMHNFSVF SNLTTIGGRS LYNRCFSLLI MKNLNVTSLG FRSLKEISAG | |
| Erb4 PPNMTDFSVF SNLVTIGGRV LYS.GLSLLI LKQQGITSLO FQSLKEISAG | |

| | | | | | | |
|------|------------|------------|-------------|----------------|------------|---------|
| Egfr | PENRTDLHAF | ENLEIIRGRT | KQHGGQFSLAV | VS.LNITSLG | LRSLEISDG | |
| Erb2 | PDSLPLDSVF | QNLQVIRGRI | LHNGAYSL.T | LQGLGISWLG | LRSLELGLSG | |
| | 451 | | | End L2 domain> | | 500 |
| Erb3 | RIYISANRQL | CYHHSNLNWK | VLRGPTTEERL | DIKHNRPRRD | CVA | EGKVCDP |
| Erb4 | NIYITDNSNL | CYYHTINWTT | LF.STINQRI | VIRDNRKAEN | CTA | EGMVCNH |
| Egfr | DVIISGNKNL | CYANTINWKK | LF.GTSGQKT | KIISNRGENS | CKA | TGQVCHA |
| Erb2 | LALIHNNTHL | CFVHTVPWDQ | LFRNP.HQAL | LHTANRPEDE | CVG | EGLACHQ |
| | 501 | | | | | 550 |
| Erb3 | LCSSGGCWGP | GPGQCLSCRN | YSRGGVCVTH | CNFLNGEPRE | FAHEAECFSC | |
| Erb4 | LCSSDGCWGP | GPDQCLSCRR | FSRGRICIES | CNLYDGEFRE | FENGSIQVEC | |
| Egfr | LCSPEGCWGP | EPRDCVSCRN | VSRGECVDK | CKLLEGEFRE | FVENSECIQC | |
| Erb2 | LCARGHCWGP | GPTQCVNCSQ | FLRGQECVEE | CRVLQGLPRE | YVNARHCLPC | |
| | 551 | | | | | 600 |
| Erb3 | HPECQPMG | TATCNGSGSD | TCAQCAHFRD | GPHCVSSCPH | GVLGA.KGP. | |
| Erb4 | DPQCEKMEDG | LLTCHGPGPD | NCTKCSHFCD | GPNCVEKCPD | GLQGA.NSF. | |
| Egfr | HPECLPQAMN | I.TCTGRGPD | NCIQCAHYID | GPHCVKTCPA | GVMGENNTL. | |
| Erb2 | HPECQPQN.G | SVTCFGPEAD | QCACAHYKD | PPFCVARCPS | GVPDLSYMP | |
| | 601 | | | | | 649 |
| Erb3 | IYKYPDVQNE | CRPCHENCTQ | GCKGPELQDC | L.....GQT. | | |
| Erb4 | IFKYADPDRE | CHPCHPNCTQ | GCNGPTSHDC | IYYPTWGHST | LPQHARTPL | |
| Egfr | VWKYADAGHV | CHLCHPNCTY | GCTGPGLEG | PTNGPKIPS. | | |
| Erb2 | IWKFPDEEGA | CQPCPINCTH | SCVDLDDKGC | PAEQRASPLT | S..... | |

Figure 15. Classification of Cys-rich modules

C2-4 denote modules with the 1-3/2-4 double disulphide bond connections.
C1-2 for the single disulphide bonded modules and
C1-2t for stabilised beta turn.

First Cys-rich region C2-4 modules

| | | 1 | 2 | 3 | 4 | | |
|--------|-----|----------------------------------|---------|-----|---|-------|--|
| Hlgf1r | 152 | CPGTMEEKPM-CEKTTINHEYNYRCWTTNRC | QKM | 184 | | (1st) | |
| Hlr | 159 | CPGTAKGKTH-CPATVINGQEVERCWTHSHC | QKV | 191 | | (1st) | |
| Hlrr | 154 | CPGV/LGAAGEPCAKTTFSGHTDYRCWTSCHC | QRV | 187 | | (1st) | |
| Egfr | 156 | COPSCPNG-SCWGAG-EENC | QKLTKEI | 190 | | (1st) | |
| hErb2 | 174 | CSPHCKGS-RCWGES-SEDC | QSLTRTV | 198 | | (1st) | |
| hErb3 | 157 | CHEVCKG--RCWGP-SEDC | QTLTKTI | 190 | | (1st) | |
| hErb4 | 157 | CHKSGTG--RCWGP-ENHC | QTLTRTV | 190 | | (1st) | |
| | | | | | | | |
| Hlgf1r | 195 | CPSTGGK-RACEN---NEC | | 200 | | (2nd) | |
| Hlr | 192 | CPTICKS-HGCTAE---GLC | | 207 | | (2nd) | |
| Hlrr | 198 | CP--CPHGMACTAR---GEC | | 202 | | (2nd) | |
| Egfr | 191 | CAQQCSG--RCRGKS-PSDC | | 207 | | (2nd) | |
| hErb2 | 199 | CAGGCA---RCKGPL-PTDC | | 214 | | (2nd) | |
| hErb3 | 191 | CAQQCNG--HCEGPH-PNQC | | 207 | | (2nd) | |
| hErb4 | 191 | CAEQCDG--RCYGPY-VSDC | | 207 | | (2nd) | |
| | | | | | | | |
| Hlgf1r | 201 | CHSECLG--SCSA2DNDTAC | VA | 220 | | (3rd) | |
| Hlr | 208 | CHSECLG--HCSQPD0PTKC | VA | 227 | | (3rd) | |
| Hlrr | 203 | CHTECLG--GCSQPEDPRAC | VA | 222 | | (3rd) | |
| Egfr | 209 | CHNQCAA--GCTGPR-ESDC | LV | 226 | | (3rd) | |
| Erb2 | 215 | CHEQCAA--GCTGPK-HSDC | LA | 233 | | (3rd) | |
| hErb3 | 208 | CHSECLG--GCSGPQ-DTDC | FA | 226 | | (3rd) | |
| hErb4 | 208 | CHRECLG--GCSGPK-DTDC | FA | 226 | | (3rd) | |

C1-2 modules

| | | | | | |
|--------|-----|------------------------------|-------|-----|-------|
| Hlgfir | 111 | CRNRY---YAGVC | VRA | 233 | (4th) |
| Hlr | 109 | CRNRY---LDGRG | VEC | 240 | (4th) |
| Hlrr | 103 | CRNRY---EQGAC | LWA | 236 | (4th) |
| Egfr | 107 | CRNER---DEATC | KDT | 239 | (4th) |
| hErb2 | 114 | CRNRY---HSGIC | ELH | 246 | (4th) |
| hErb3 | 107 | CRNRY---DSBAC | VRA | 239 | (4th) |
| hErb4 | 107 | CRNRY---DSBAC | WQ | 239 | (4th) |
| Hlgfir | 114 | CPNDRREFEDWRC | WDRF | 251 | (5th) |
| Hlr | 111 | CPNRYVHFQDWRC | WDFP | 258 | (5th) |
| Hlrr | 106 | CPNRYVHFQESWRC | WTAER | 253 | (5th) |
| Egfr | 140 | CPFLMLNHTTYQNDNPEGKYSFGATC | VKK | 270 | (5th) |
| hErb2 | 147 | CPALVTNITDTFESHNPESGRITFGASC | VTA | 277 | (5th) |
| hErb3 | 140 | CPQPLVYHKLTFQLEPNHTKIQYGGVC | VAS | 270 | (5th) |
| hErb4 | 140 | CPQTEVYNHTTFQLEHNEAKITYGAF | VKK | 270 | (5th) |
| Hlgfir | 152 | CAVLSAESSDSEG.....FVIHD.GEC | NQE | 276 | (6th) |
| Hlr | 159 | CCQ.LHRKCKNRRQSGCHQYVIHN.NKC | ISE | 287 | (6th) |
| Hlrr | 154 | CAE.LHSVPSRAST.....FGIHQ.GEC | LAQ | 276 | (6th) |
| Egfr | 171 | CPNRYV/TDHGSC | VRA | 296 | (6th) |
| hErb2 | 179 | CPNRYVUSTDVGSC | TLV | 293 | (6th) |
| hErb3 | 171 | CPNRYV/LDQTS | VRA | 296 | (6th) |
| hErb4 | 171 | CPNRYV/LDSSC | VRA | 296 | (6th) |
| Hlgfir | 177 | CPSS.FTRNGSQ-SHNC | IP | 293 | (7th) |
| Hlr | 199 | CPSS.VTNGSH--GLC | TP | 303 | (7th) |
| Hlrr | 173 | CPSS.FTRNGS--SIFC | HK | 293 | (7th) |
| Egfr | 147 | CJADSVENE-EDGVKNC | KK | 304 | (7th) |
| hErb2 | 144 | CPNRYVTAEDPTAC | SK | 312 | (7th) |
| hErb3 | 144 | CPNRYVTAEDPTAC | SK | 312 | (7th) |
| hErb4 | 144 | CPNRYVTAEDPTAC | SK | 312 | (7th) |

C1-2t module

| | | | | |
|--------|-----|-------|-----|-------|
| Higflr | 294 | CEGPC | 298 | (8th) |
| Hlr | 304 | CLGPC | 308 | (8th) |
| Hlrr | 294 | CEGLC | 298 | (8th) |
| hEgfr | 305 | CEGPC | 309 | (8th) |
| hErb2 | 313 | CSKPC | 317 | (8th) |
| hErb3 | 304 | CGGLC | 308 | (8th) |
| hErb4 | 304 | CTDIC | 308 | (8th) |

Second Cys-rich region.**C2-4 modules**

| | | | | |
|-------|-----|--|-----|-------|
| hEgfr | 482 | CHALCSP-----EGCWGPEPRDCVS | 501 | (1st) |
| hErb2 | 490 | CHQLCAR-----GHCWGPGPTQCVN | 509 | (1st) |
| hErb3 | 481 | CDPLCSS-----GGCWGPGPGQCLS | 500 | (1st) |
| hErb4 | 481 | CNHLCSS-----DGCWGPGPDQCLS | 500 | (1st) |
| Egfr | 534 | CHPECLPQAM-NITCTGRGPDNC IQ | 557 | (4th) |
| hErb2 | 542 | CHPECQPQNG-SVTCFGPEADQC VA | 565 | (4th) |
| hErb3 | 533 | CHPECQPMEG-TATCNGSGSDTC AQ | 556 | (4th) |
| hErb4 | 533 | CDPQCEKMEDGLLTCHGPGPDNC TK | 557 | (4th) |
| hEgfr | 596 | CHPNCTY-----GCTGPGLEG C PTNGPKIPS/ | 621 | (7th) |
| hErb2 | 605 | CPINCTH-----SCVDLDDKGC PAEQRAQRASPLTS/ | 632 | (7th) |
| hErb3 | 594 | CHENCTQ-----GCKGPELQDC LGQT/ | 614 | (7th) |
| hErb4 | 595 | CHPNCTQ-----GCNGPTSHDC IYYPWTGHSTLPQHARTPL | 630 | (7th) |

C1-2 modules

| | | | | |
|-------|-----|------------------------------|-----|-------|
| hEgfr | 502 | CRNVS---RGREC VDX | 514 | (2nd) |
| hErb2 | 510 | CSQFL---RGQEC VEE | 522 | (2nd) |
| hErb3 | 501 | CRNYS---RGGVC VTH | 513 | (2nd) |
| hErb4 | 501 | CRRFS---RGRIC IES | 513 | (2nd) |
| hEgfr | 515 | CKLLEGEPREFVENSEC IQ | 533 | (3rd) |
| hErb2 | 523 | CRVLQGLPREYVNARHC LP | 541 | (3rd) |
| hErb3 | 514 | CNFLNGEPREFAHEAEC FS | 532 | (3rd) |
| hErb4 | 514 | CNLYDGEFREFENGSI C VE | 532 | (3rd) |
| hEgfr | 553 | CAHYI---DGPHC VKT | 570 | (5th) |
| hErb2 | 555 | CAHYK---DPPFC V-A | 578 | (5th) |
| hErb3 | 557 | CAHFR---DGPHC V-S | 569 | (5th) |
| hErb4 | 553 | CSHFK---DGPNC VEX | 570 | (5th) |
| hEgfr | 571 | CPAGVMGENNTL-VNXYADAGHYC HL | 595 | (6th) |
| hErb2 | 573 | CPSGVXPDL SYMPIWKFPEEGAC QP | 604 | (6th) |
| hErb3 | 570 | CPHGVLGAKG---PIYKYPDVQNEC RP | 593 | (6th) |
| hErb4 | 571 | CPDGLQGANS---FIFKYADPDREC HP | 594 | (6th) |

See Pattern is:

IR family: C2-4, C2-4, C2-4, C1-2, C1-2, C1-2, C1-2, C1-2t
EGFR family: 1st C2-4, C2-4, C2-4, C1-2, C1-2, C1-2, C1-2, C1-2t
2nd C2-4, C1-2, C1-2,
C2-4, C1-2, C1-2,
C2-4

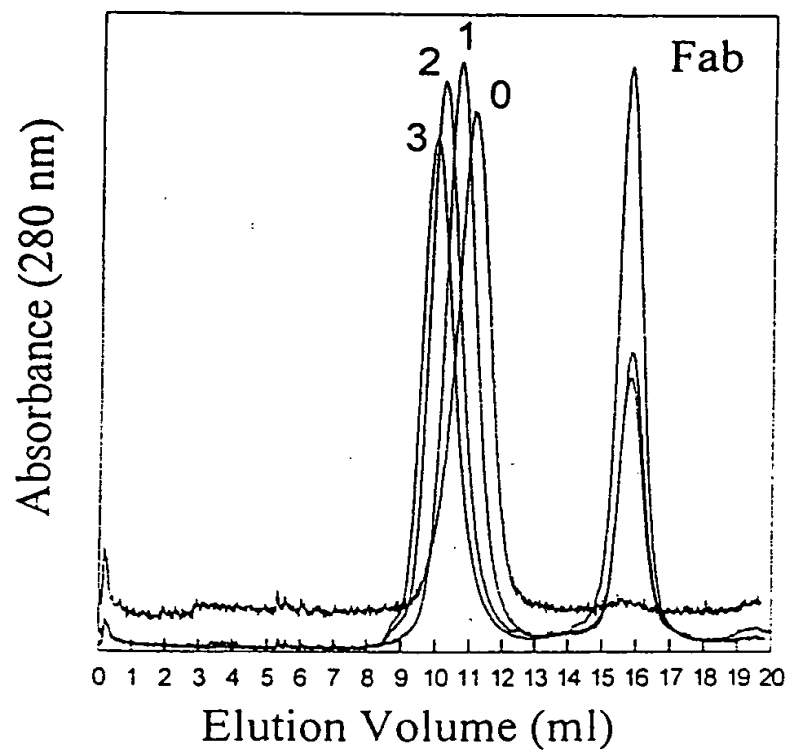
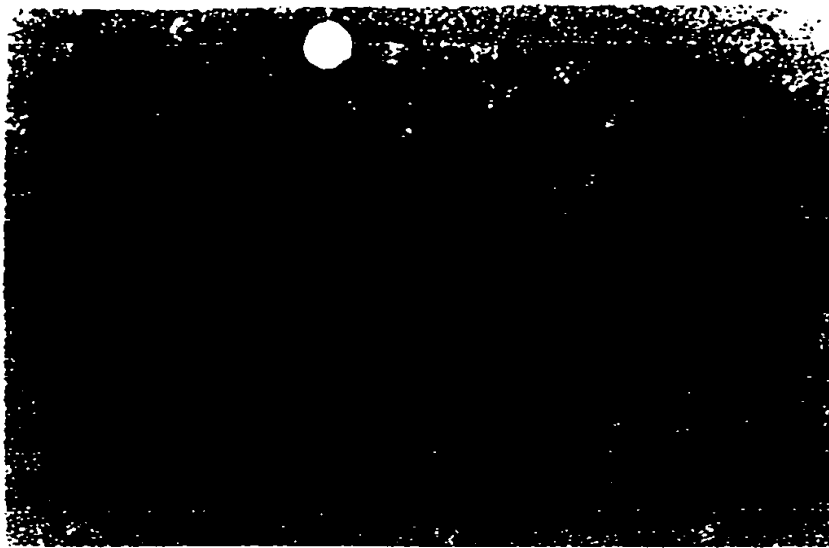


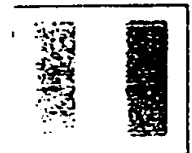
Figure 16



(a)



Figure 17



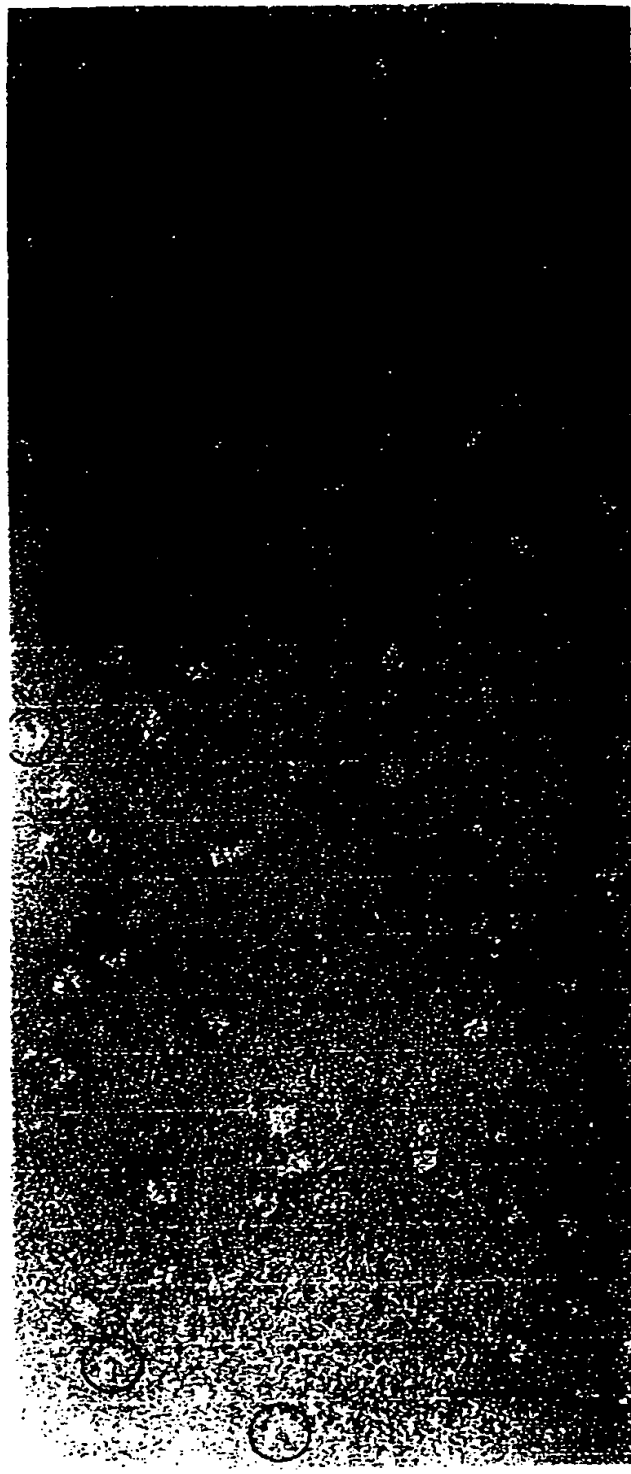


Figure 18

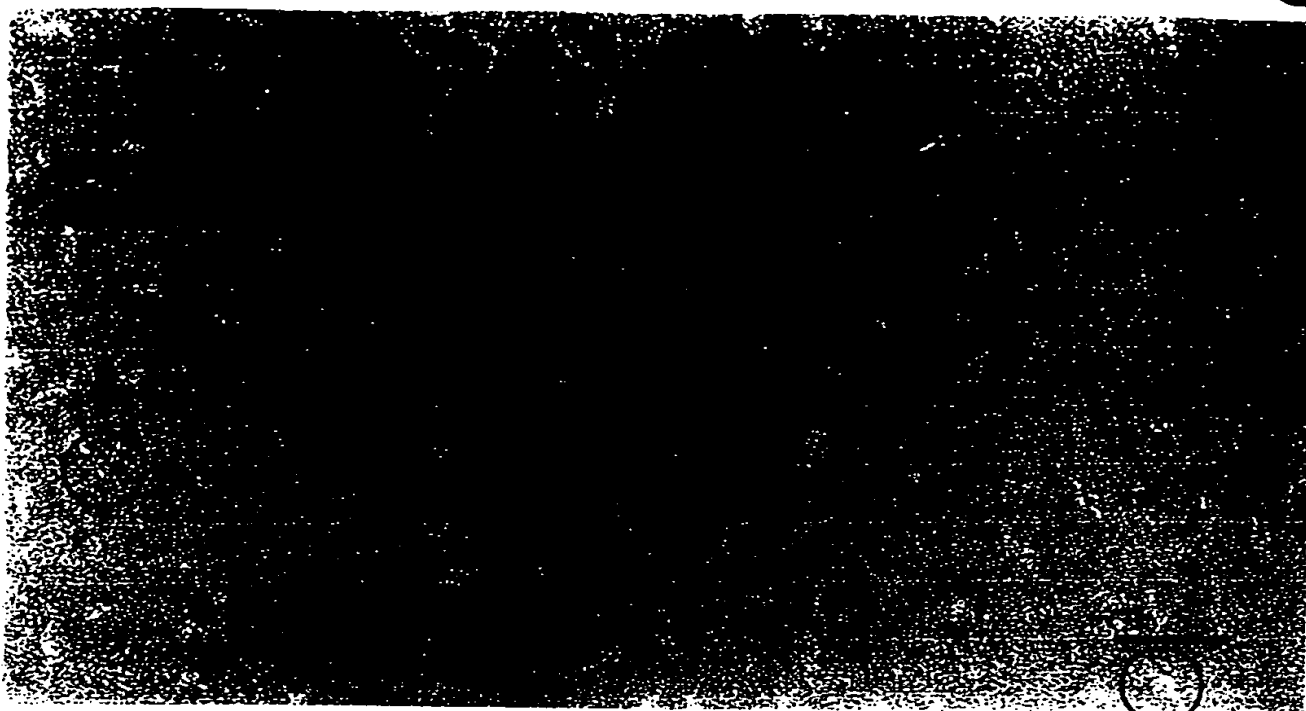


Figure 19

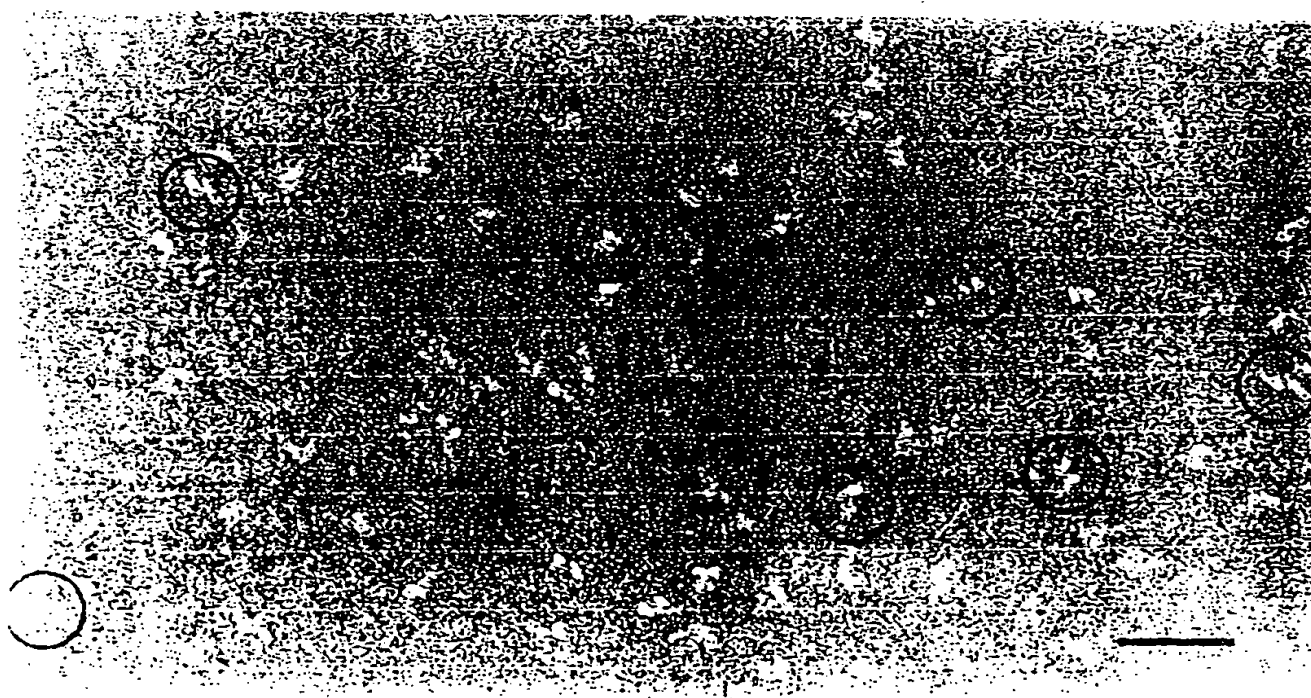
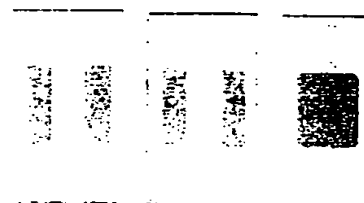


Figure 20

(a)



(b)

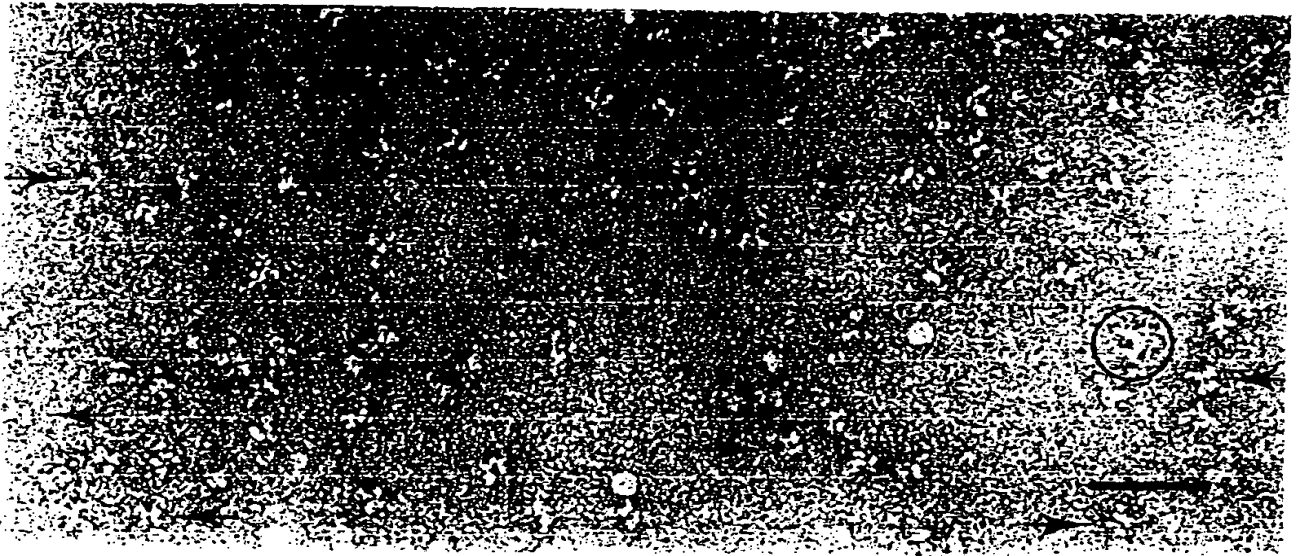


Figure 21



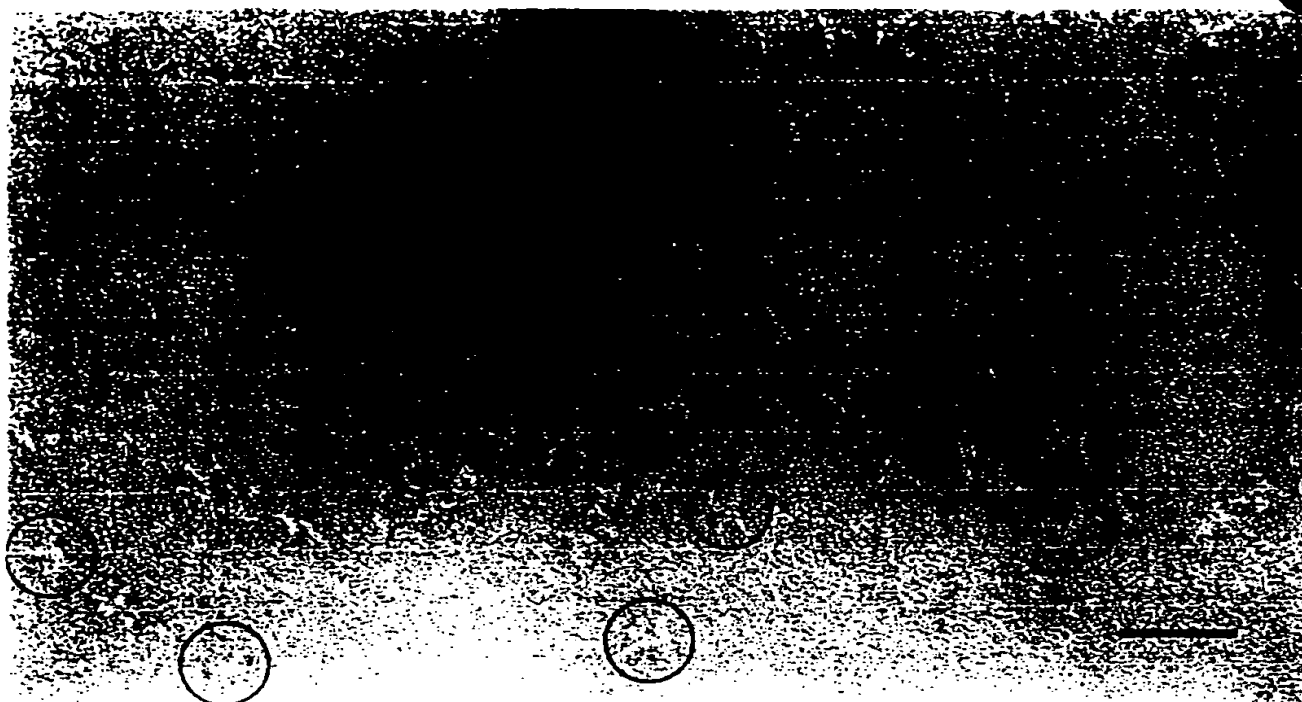


Figure 22

11

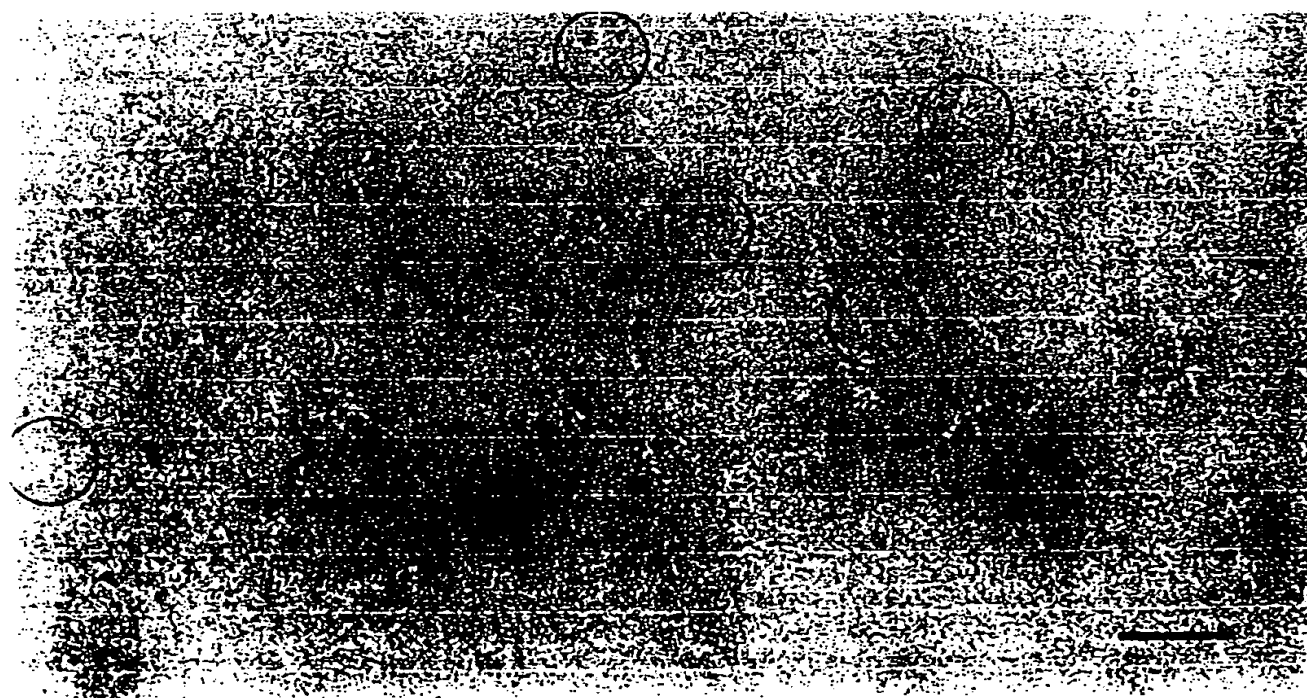


Figure 23